Using Diffusion Monte Carlo to Probe Rotationally Excited States

Andrew S. Petit and Anne B. McCoy
The Ohio State University

Putting Diffusion Monte Carlo Onto a Carousel

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Why Diffusion Monte Carlo (DMC)???

Highly fluxional molecules

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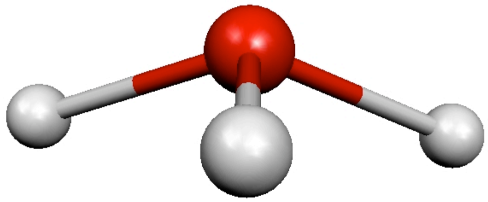

H_3O^+

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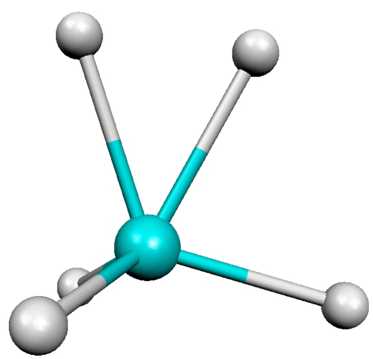
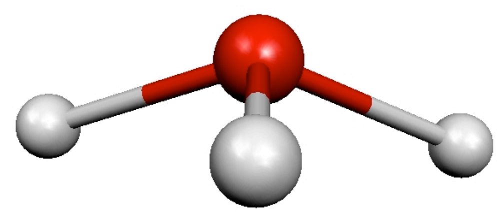


CH_5^+



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The General Diffusion Monte Carlo Methodology

$$i\hbar\frac{\partial\Psi}{\partial t} = \sum_{i=1}^{N} -\frac{\hbar^2}{2m_i}\nabla_i^2\Psi + V\Psi \qquad \Psi(t) = e^{\frac{itE_{ref}}{\hbar}}\sum_k c_k e^{\frac{-itE_k}{\hbar}}\phi_k$$

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Solution via statistical simulation!!!

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Equilibrium

$$\lim_{\tau\to\infty}\Psi(\tau)=c_0\phi_0$$

A Simple Game of Chance

Use an ensemble of *M* δ-functions (walkers) to represent *N* particle wave function

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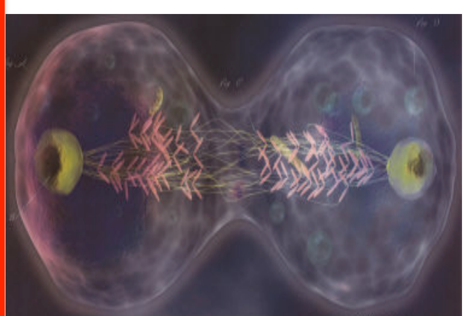

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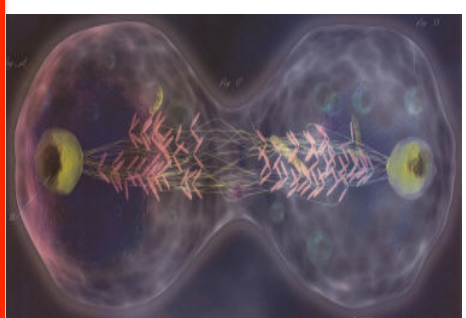

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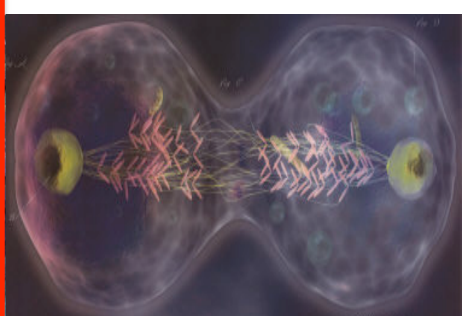

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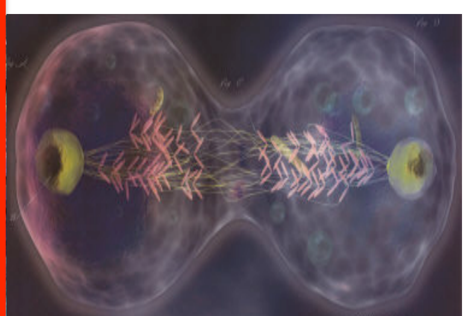
Reference energy updated every time step



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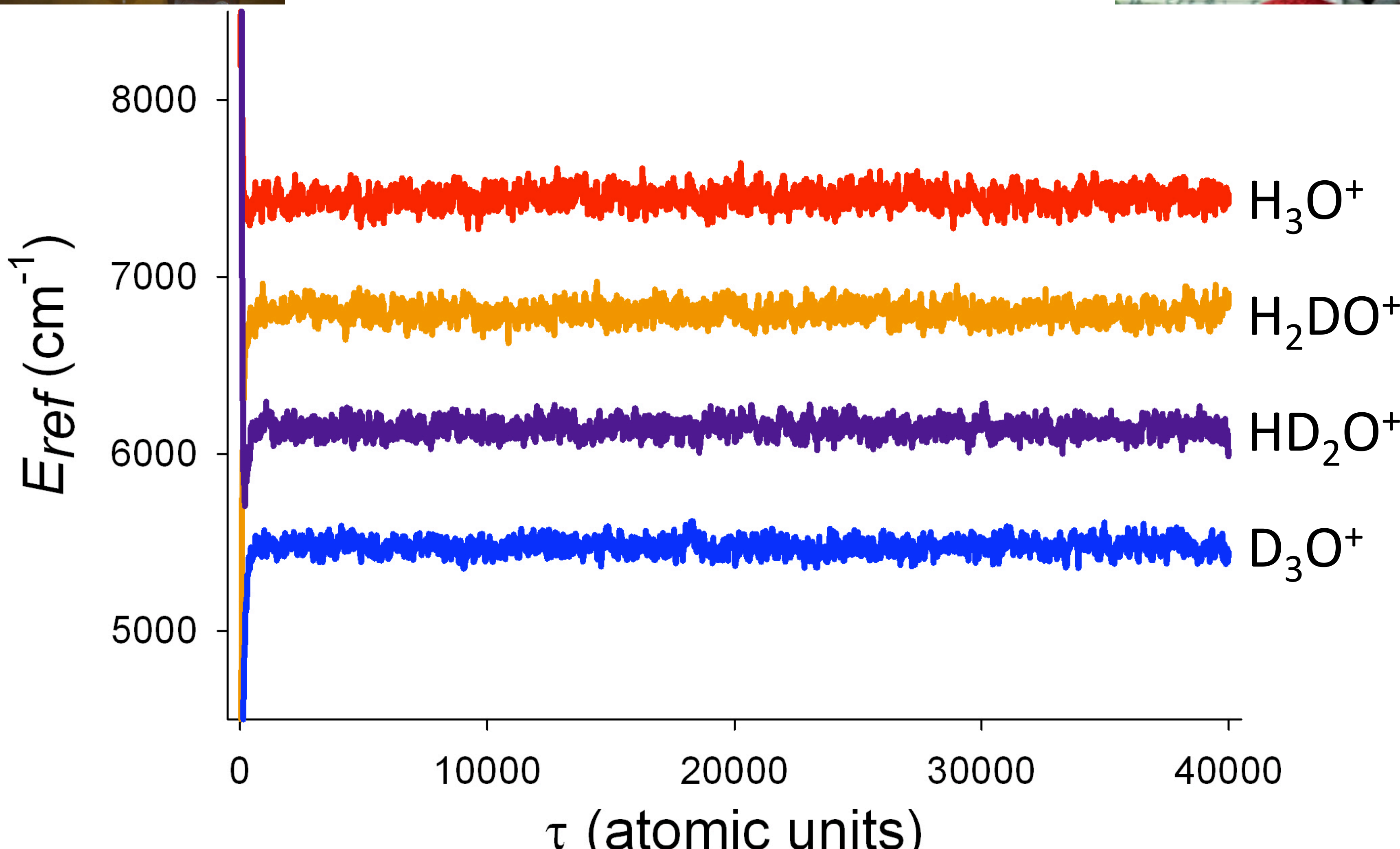
Evolution of E_{ref} with τ



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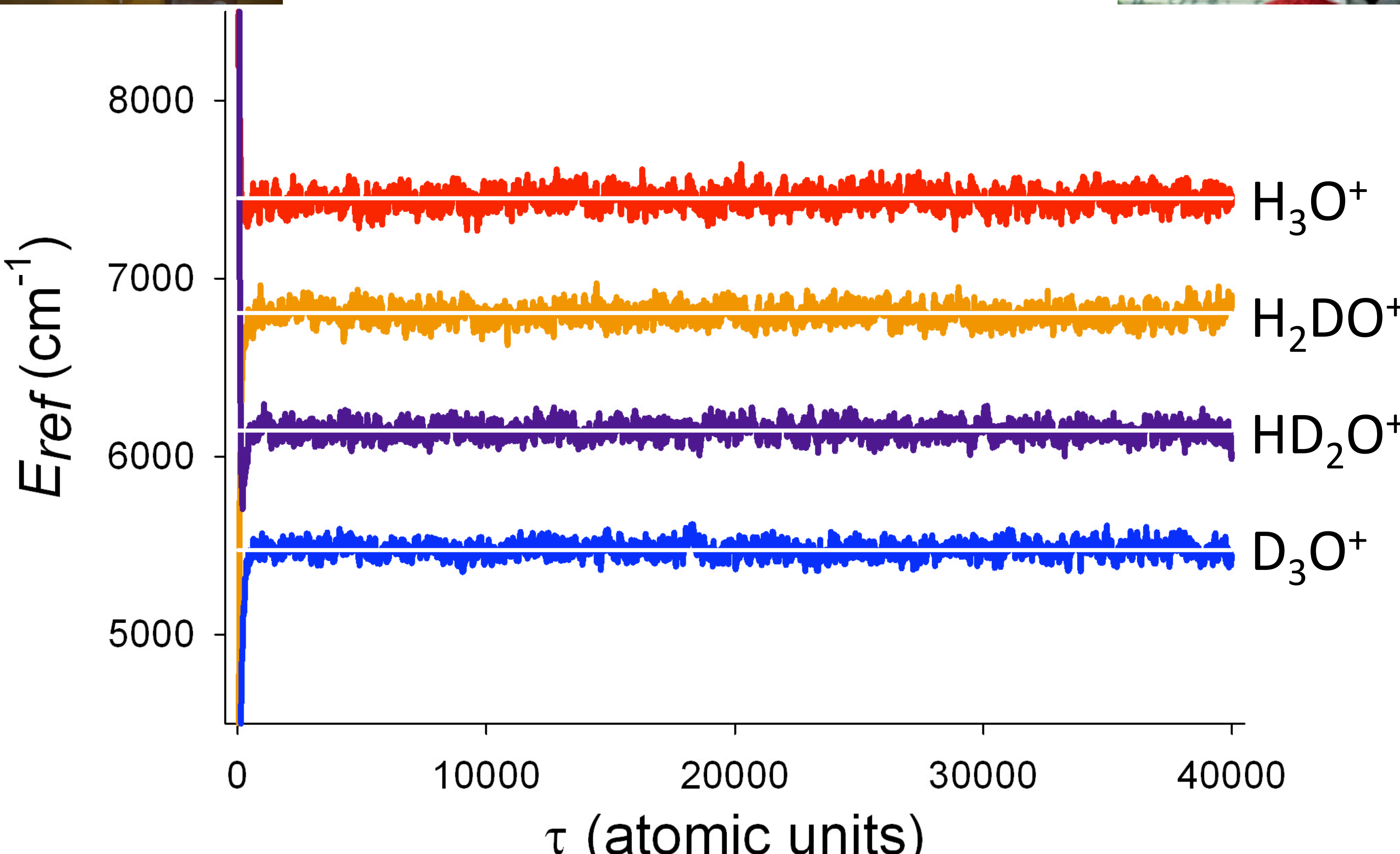

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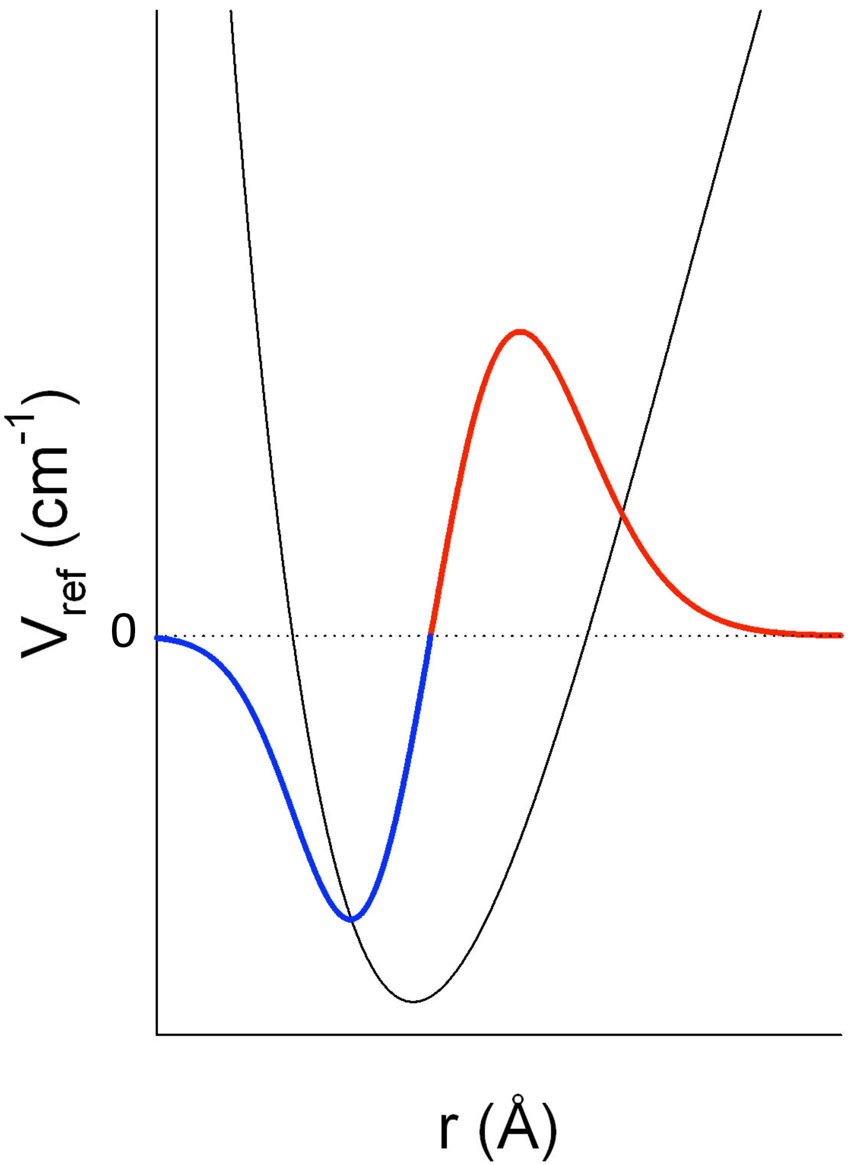
What About Excited States???

Fixed Node DMC

Assumes some knowledge of nodal surfaces



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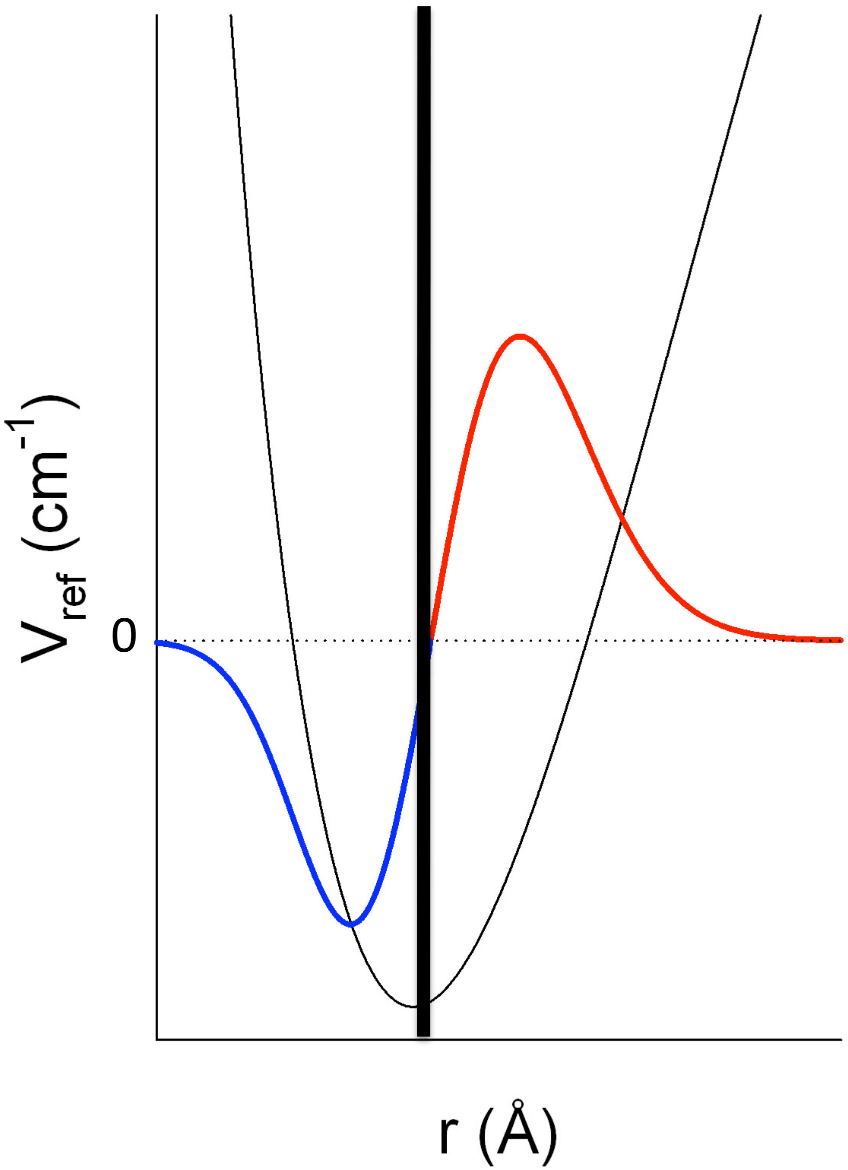

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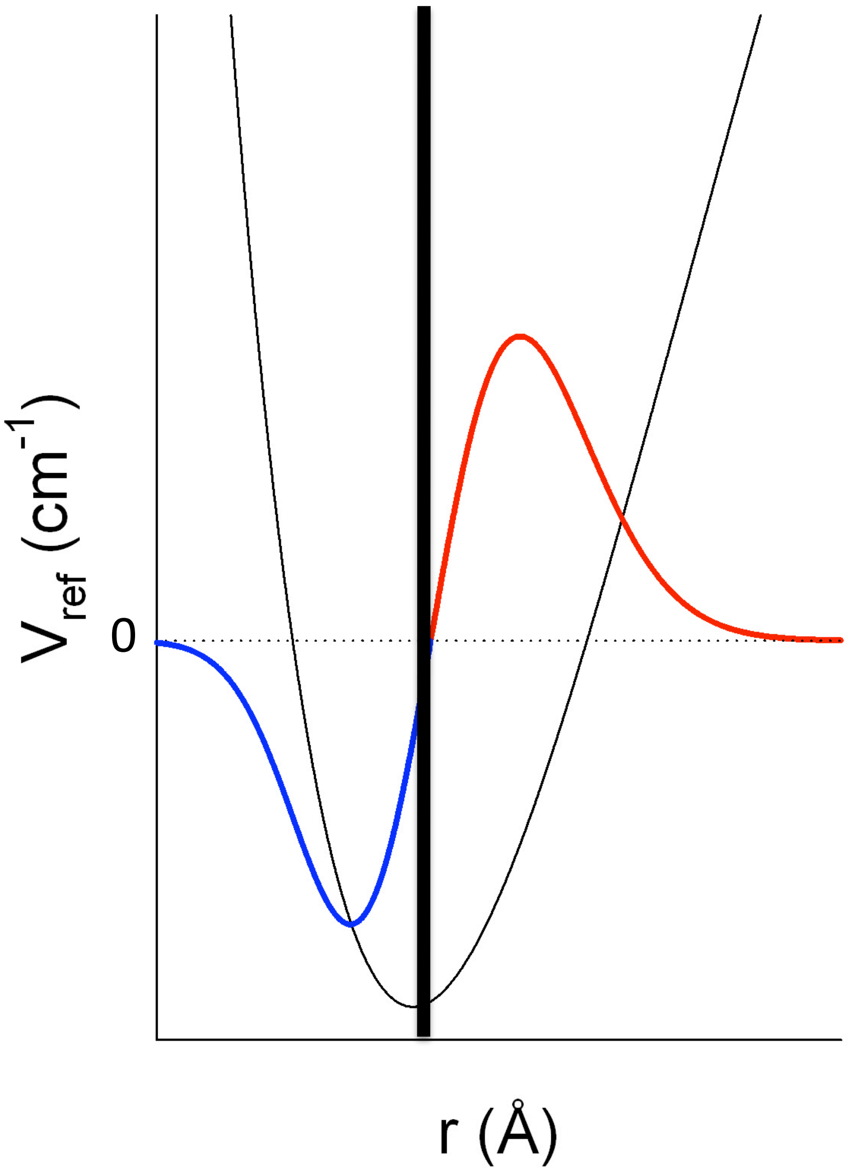

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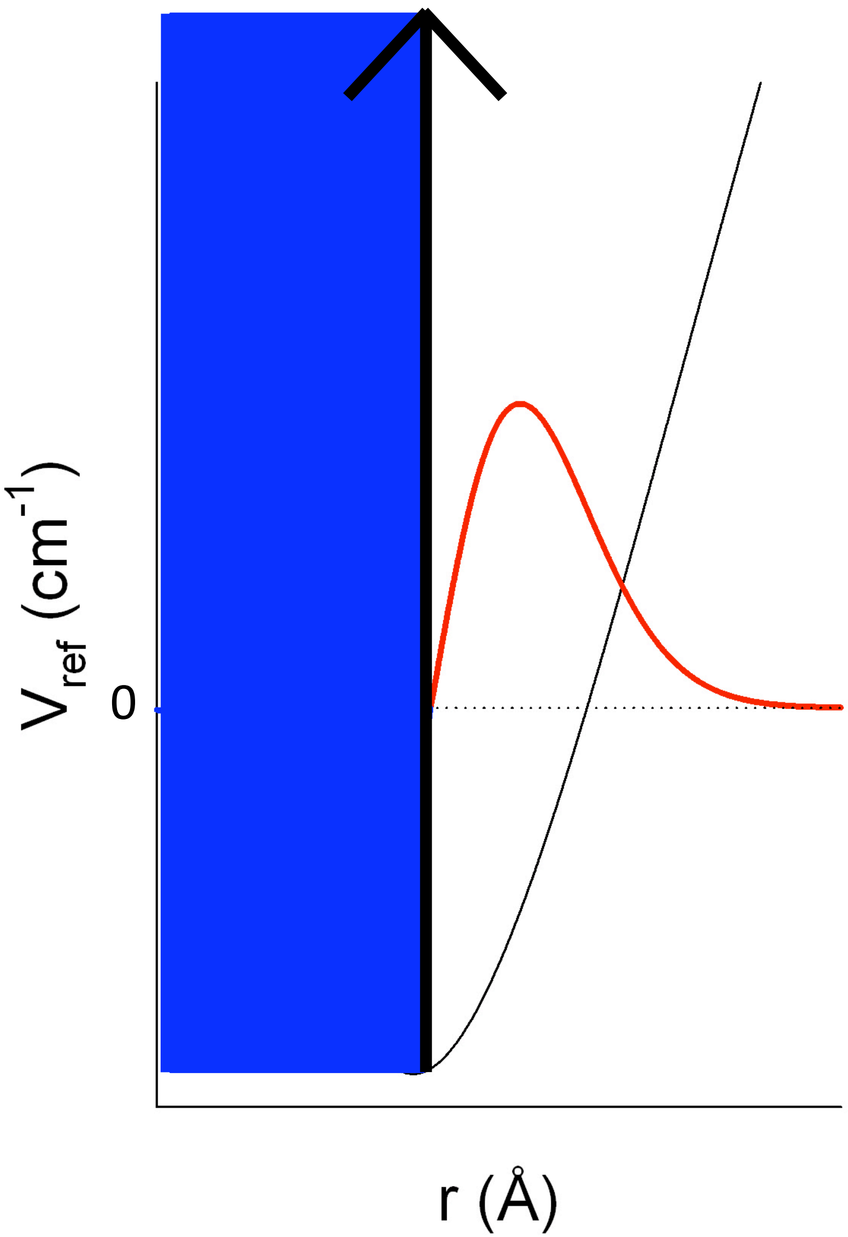

Fixed Node DMC

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Modify Hamiltonian with infinite potential placed outside of nodal region

Lowest energy state of new Hamiltonian:

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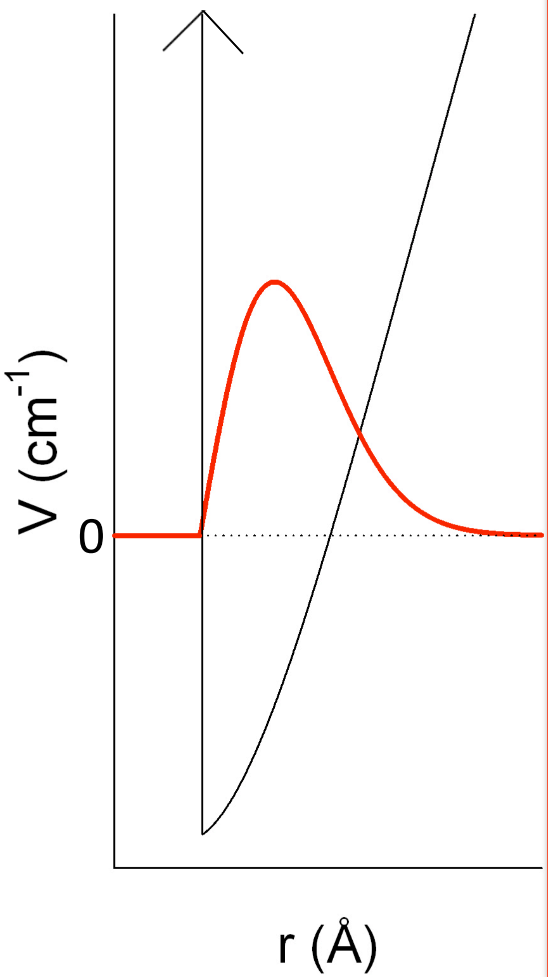

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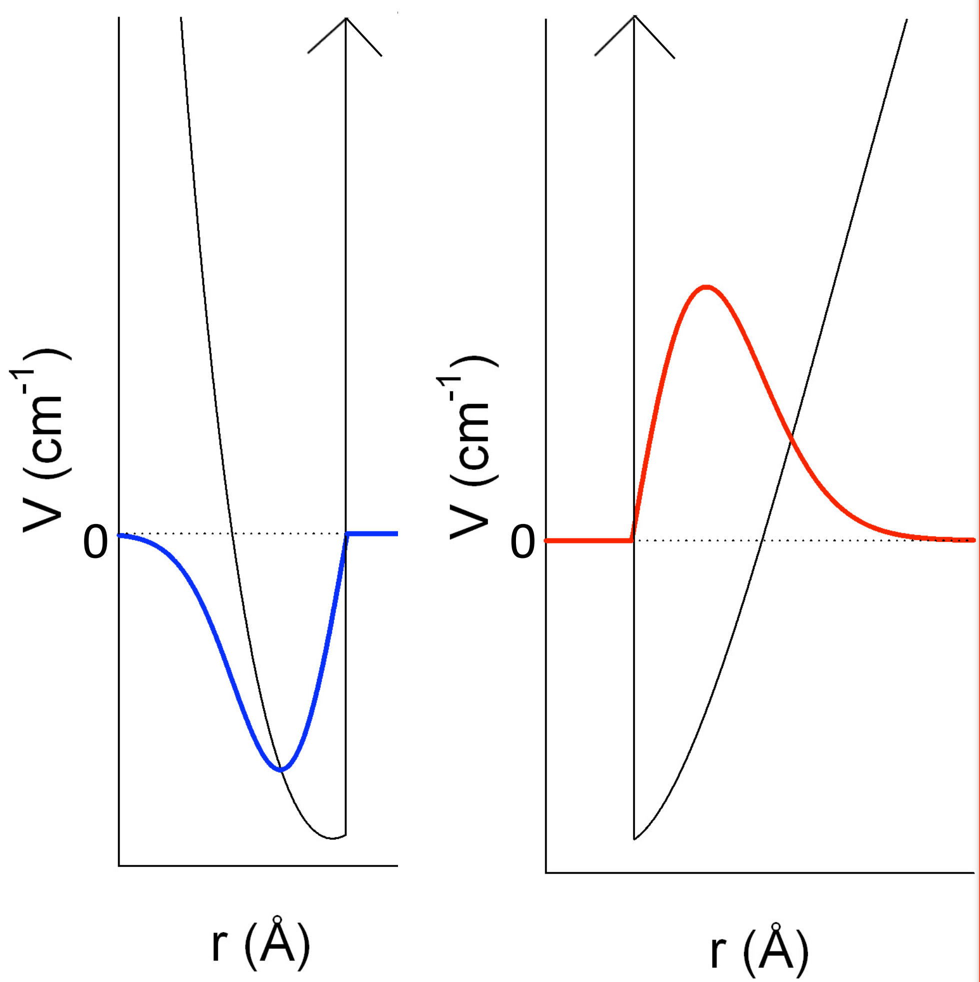

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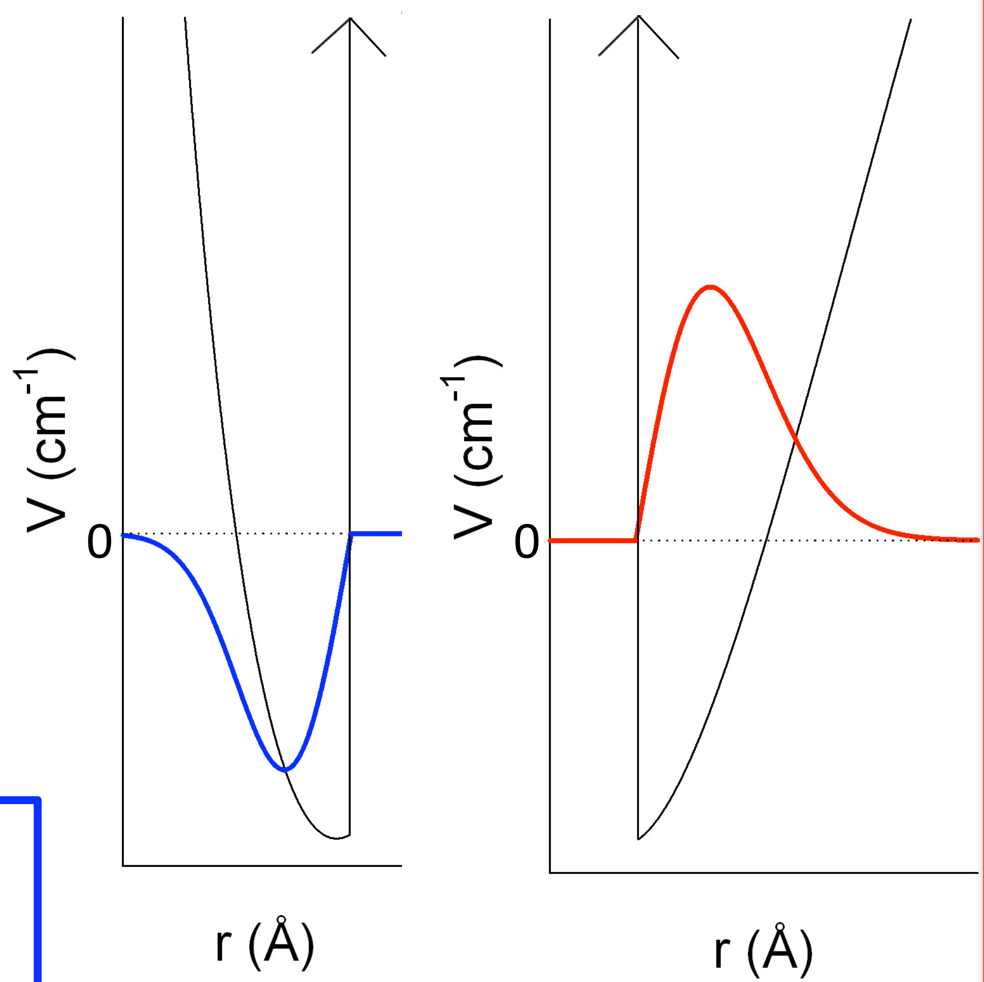
Average energies in both nodal regions must be equal



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Rotational component of wave function ONLY depends on $\{\theta, \chi, \phi\}$

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Nodal surfaces given by: $\theta = \theta_{node}$ OR $\chi = \chi_{node}$

Obtaining the Rotational Coordinates

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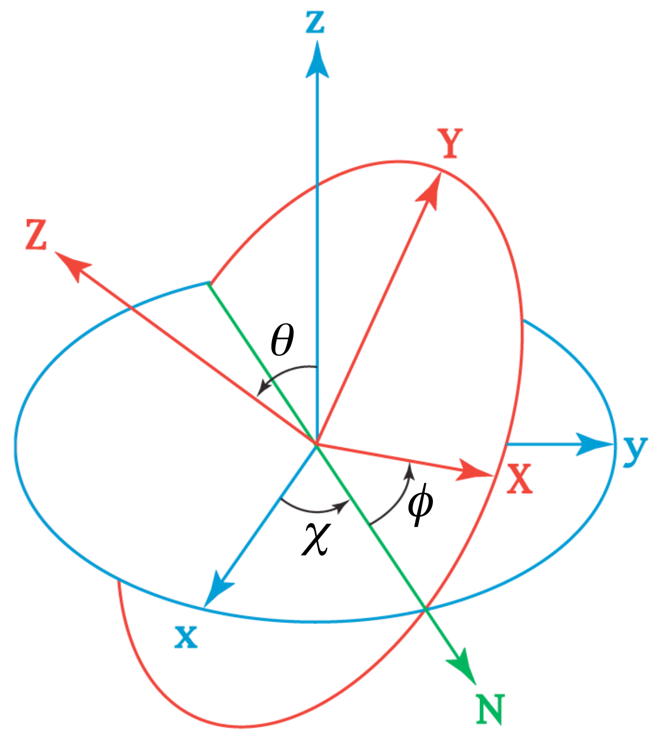

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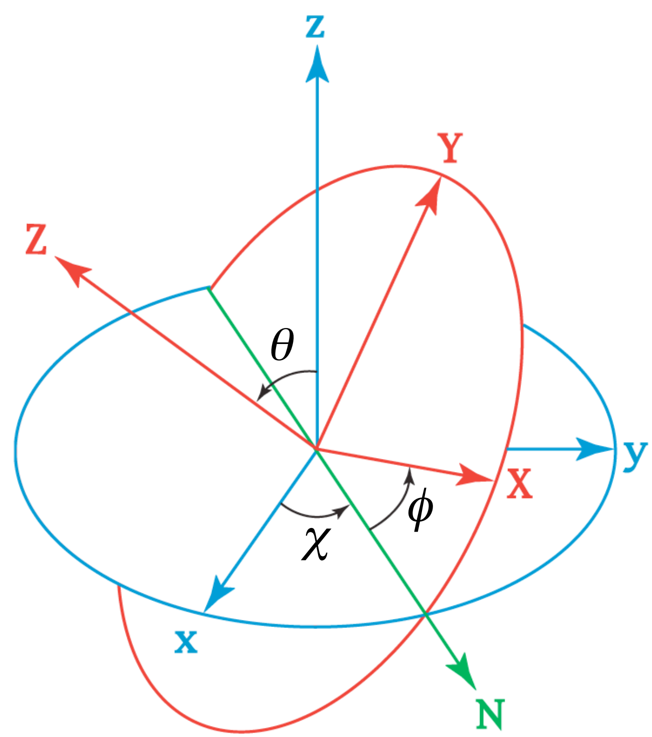

$$\begin{bmatrix} c\theta c\chi c\phi - s\chi s\phi & -c\theta s\chi c\phi - c\chi s\phi & s\theta c\phi \\ c\theta c\chi s\phi + s\chi c\phi & -c\theta s\chi s\phi + c\chi c\phi & s\theta s\phi \\ -s\theta c\chi & s\theta s\chi & c\theta \end{bmatrix}$$

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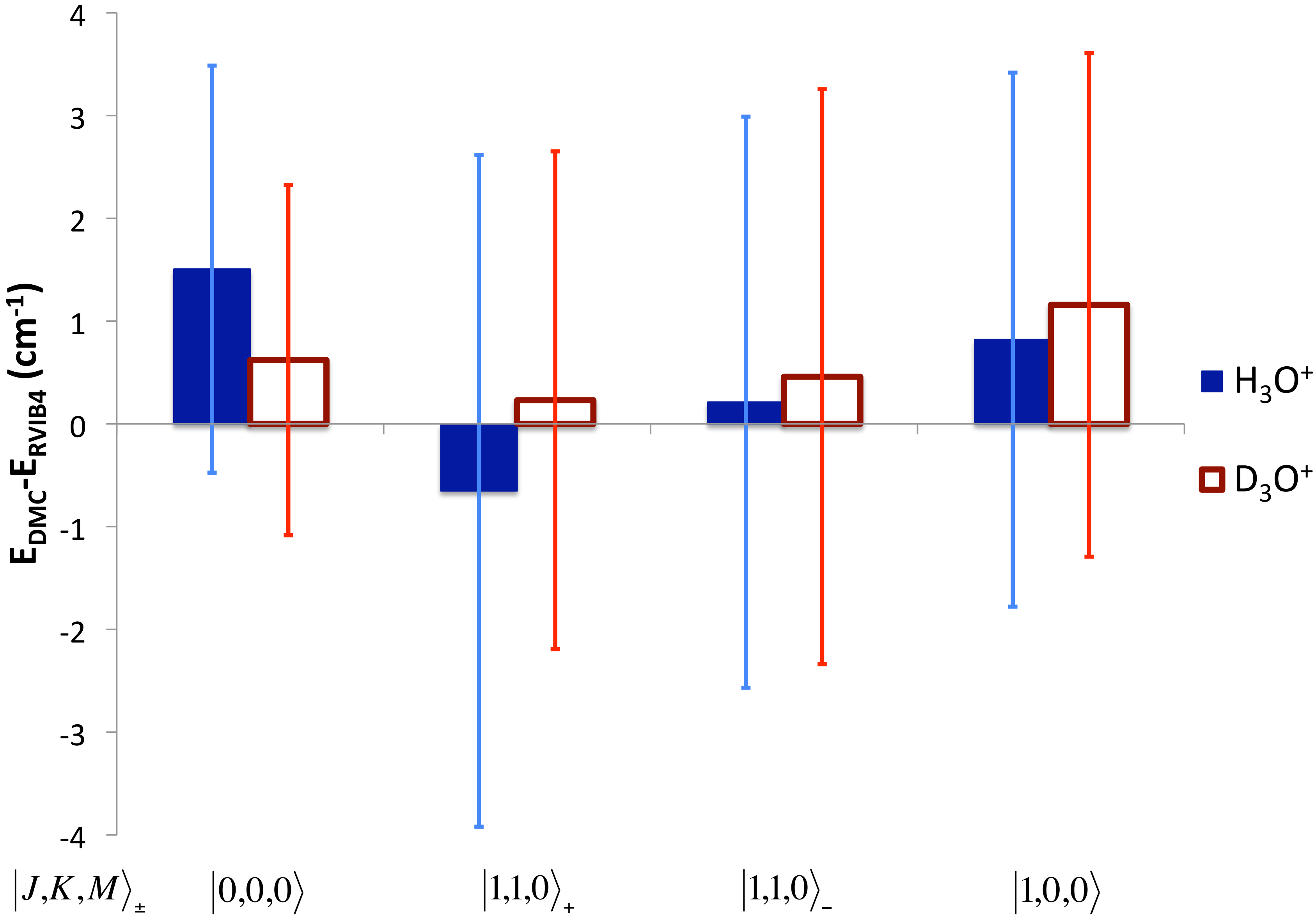
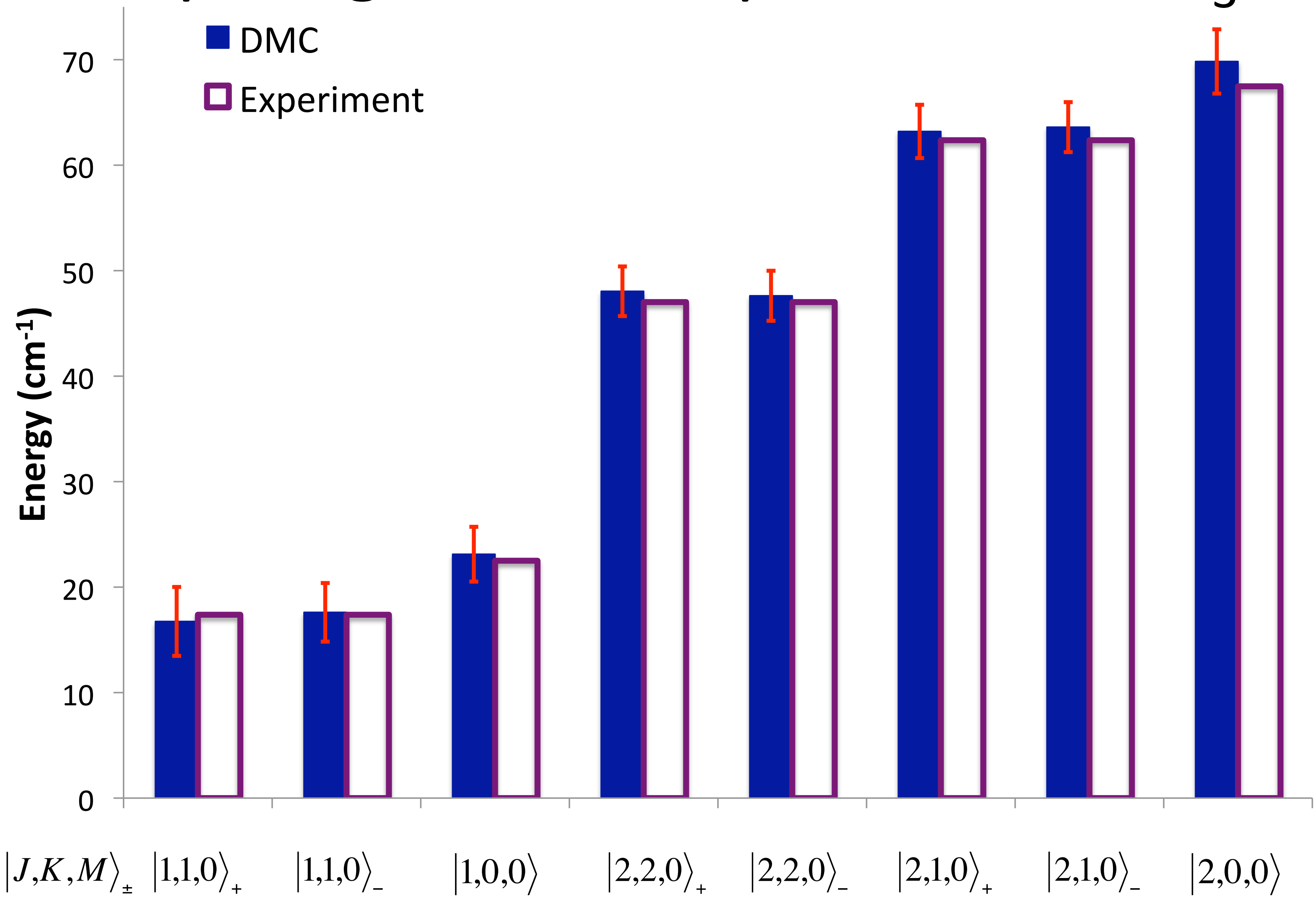
Experiment

Comparing DMC and RVIB4 Energies



Huang, X.; Carter, S.; Bowman, J.M. *J. Chem. Phys.* **2003**, *118*, 5431-5441.

Comparing DMC to Experiment for H_3O^+



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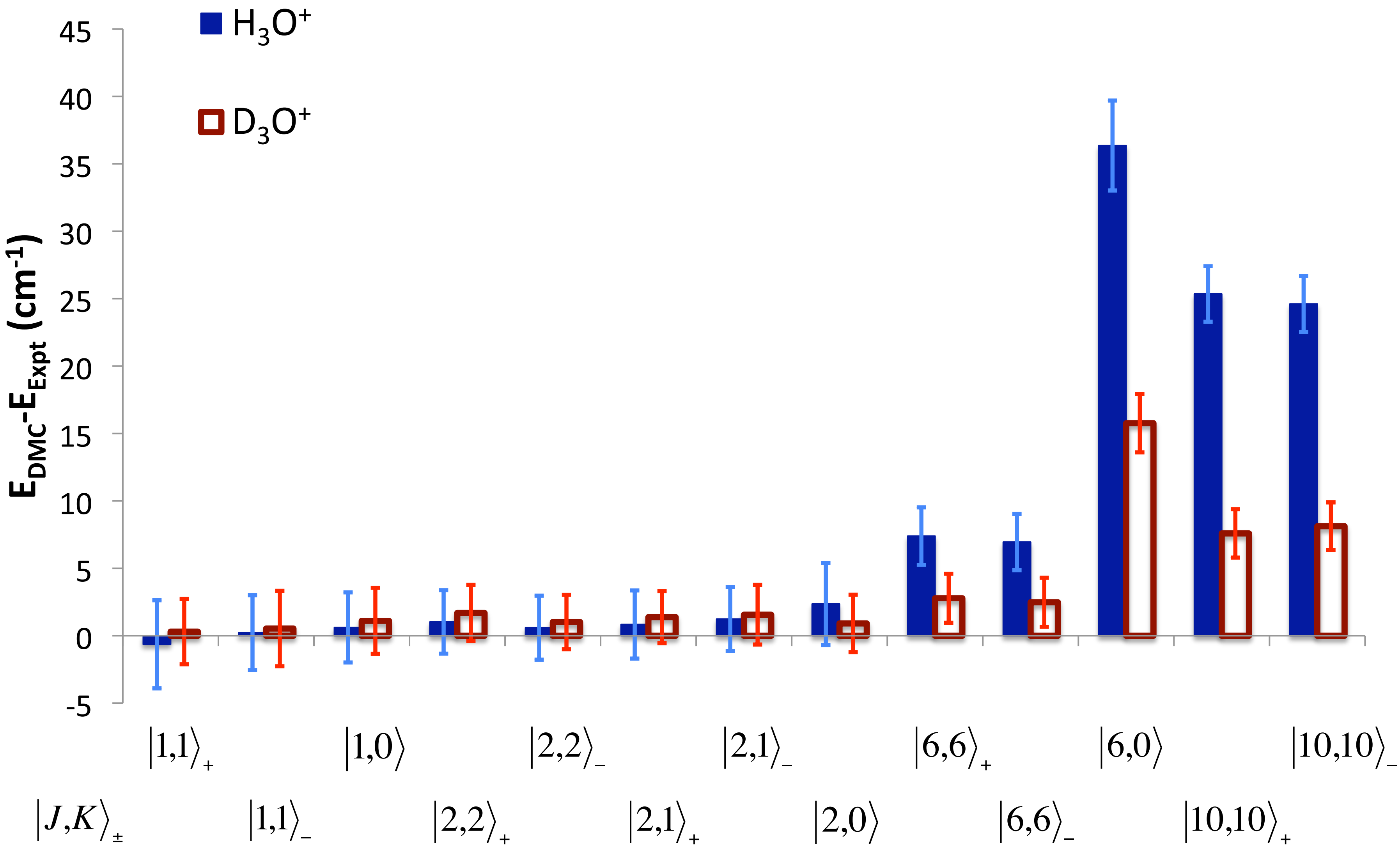

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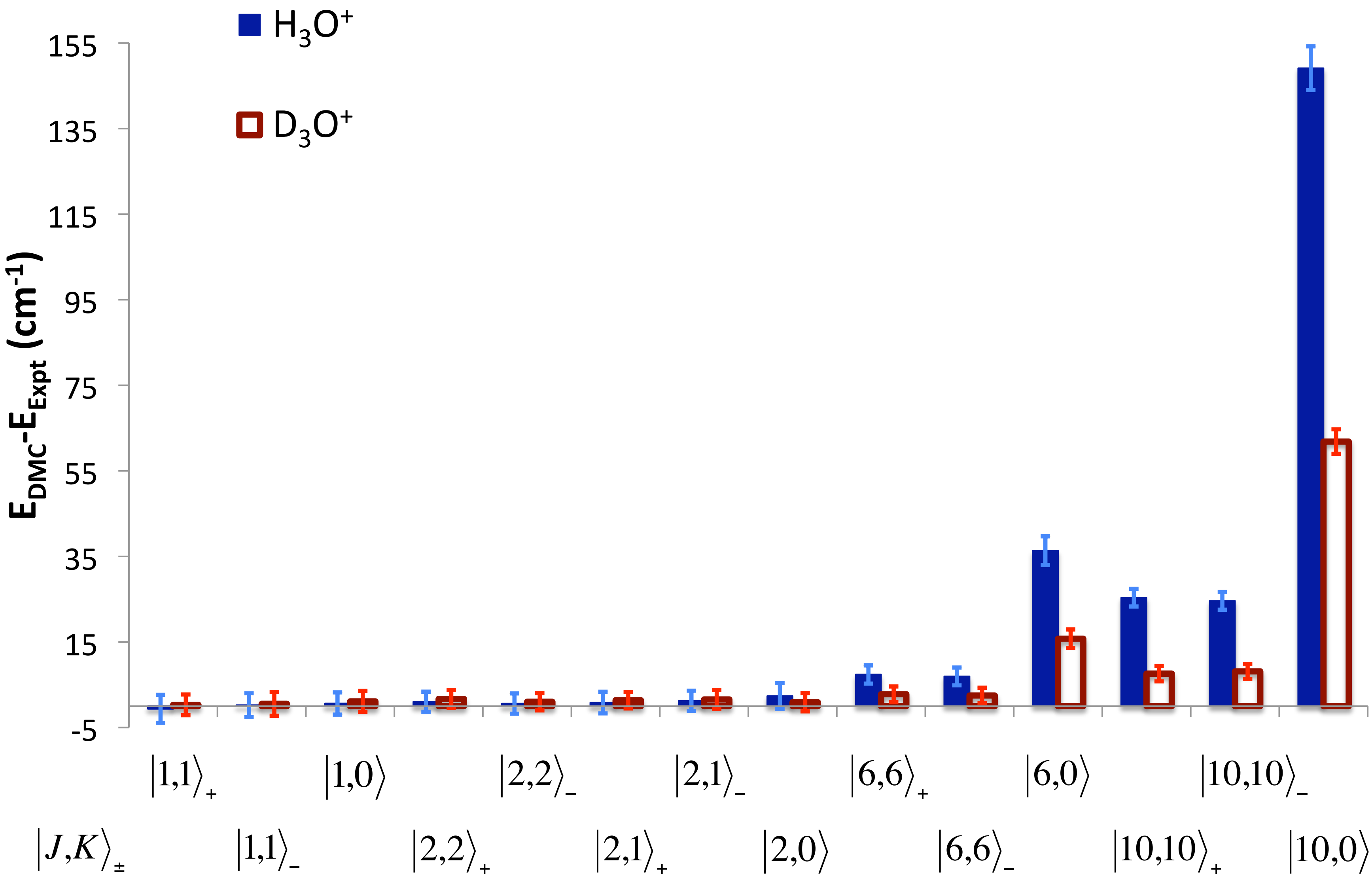

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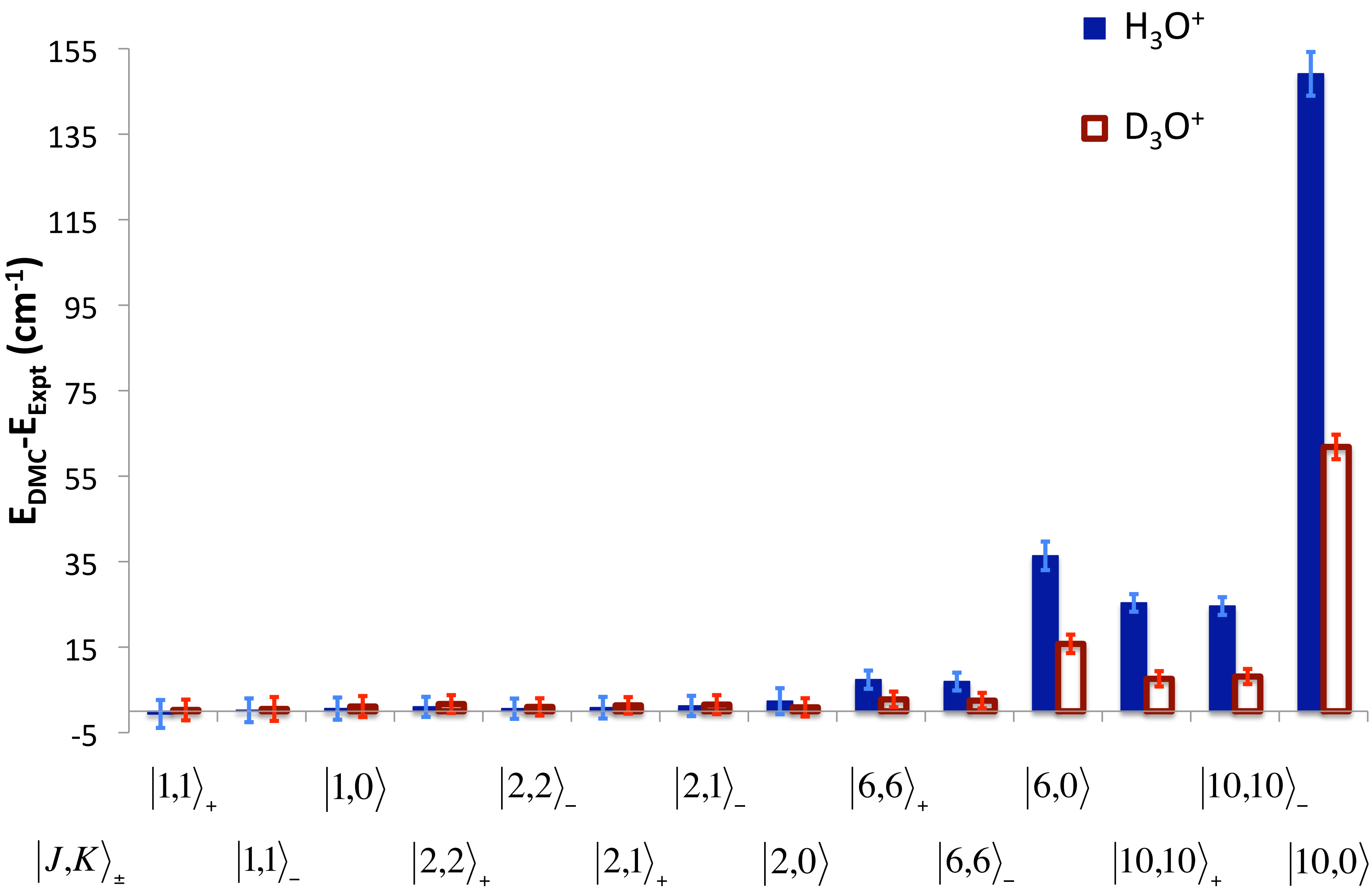
What Causes Deviations at Large J???



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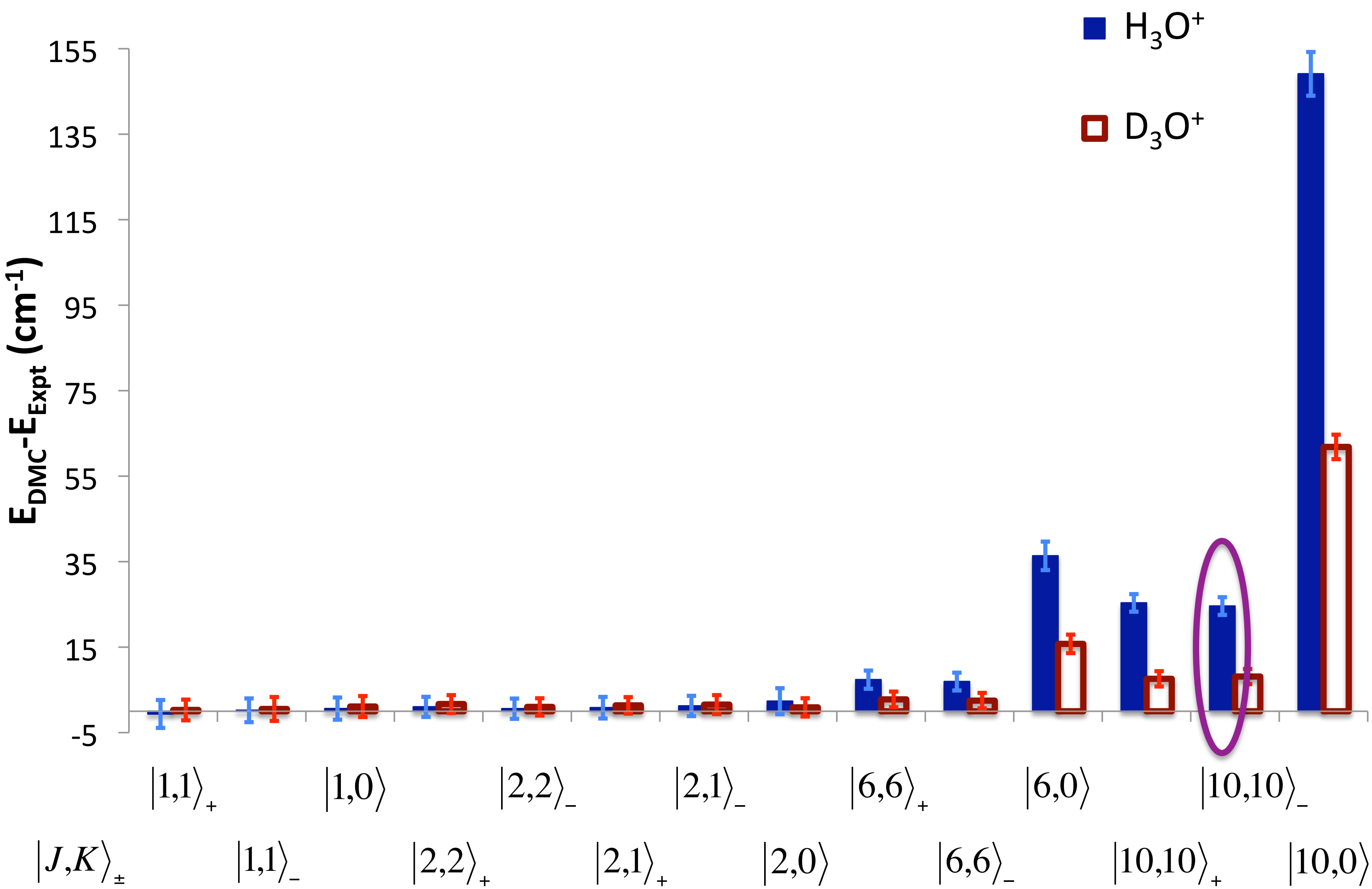

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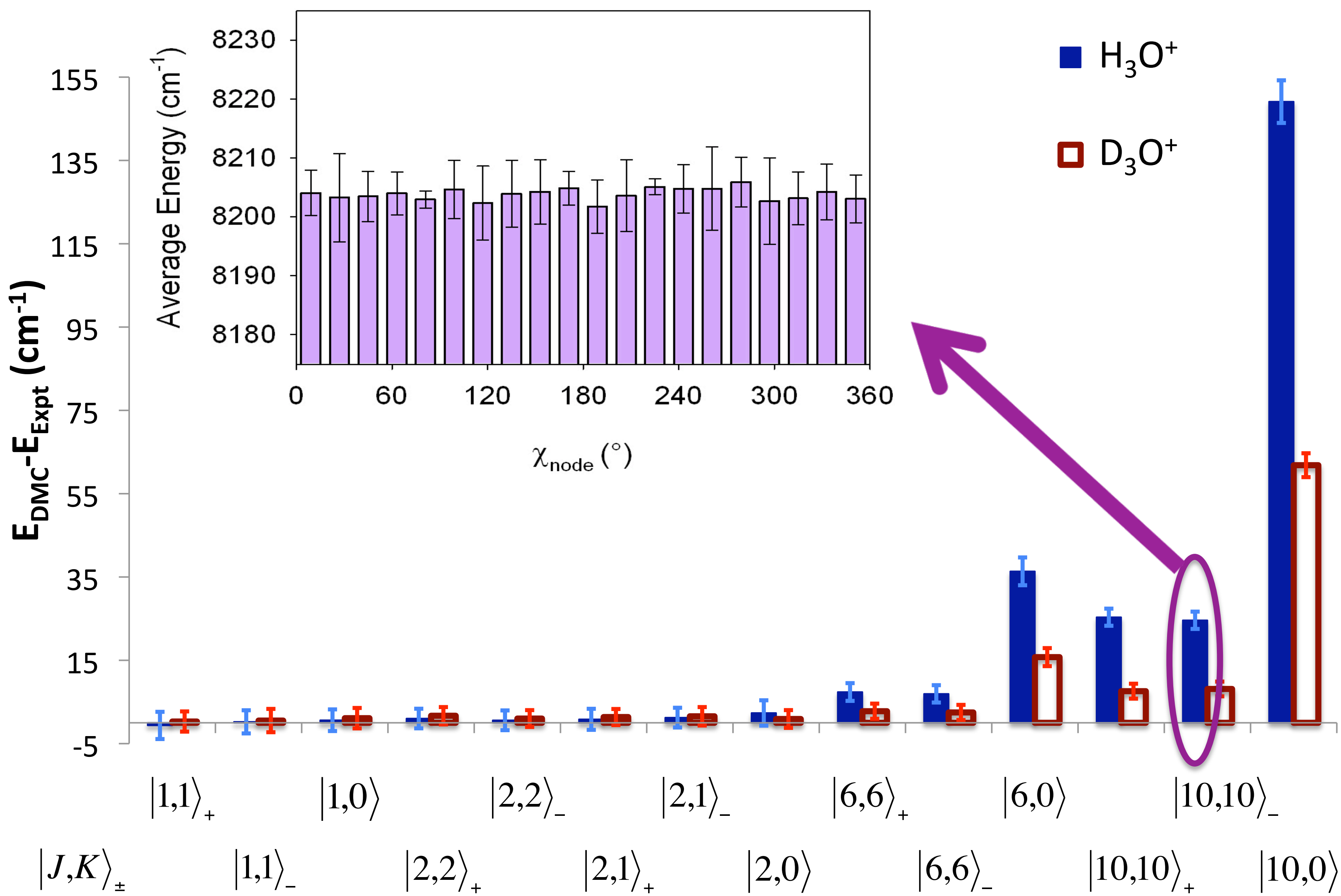

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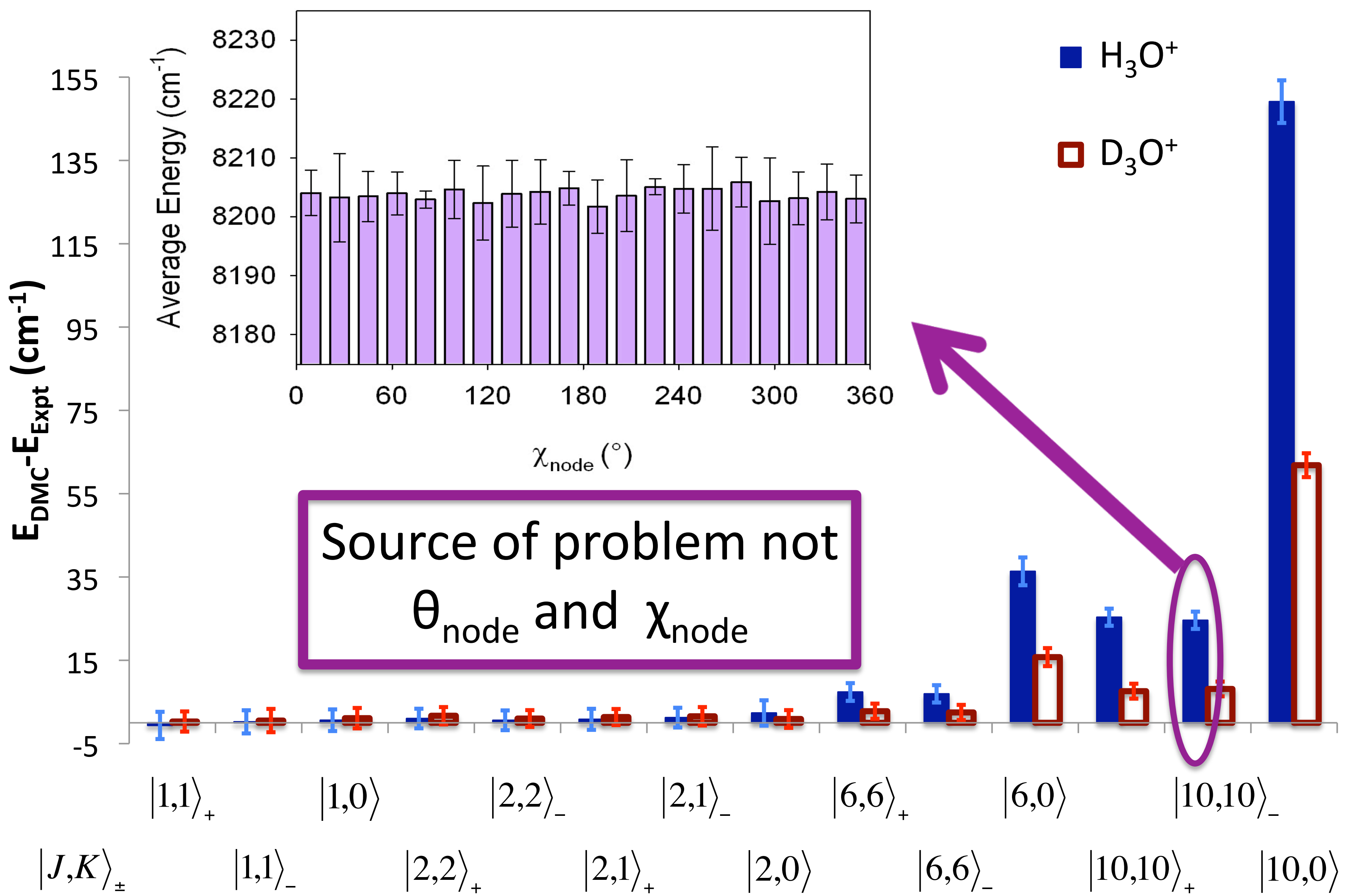

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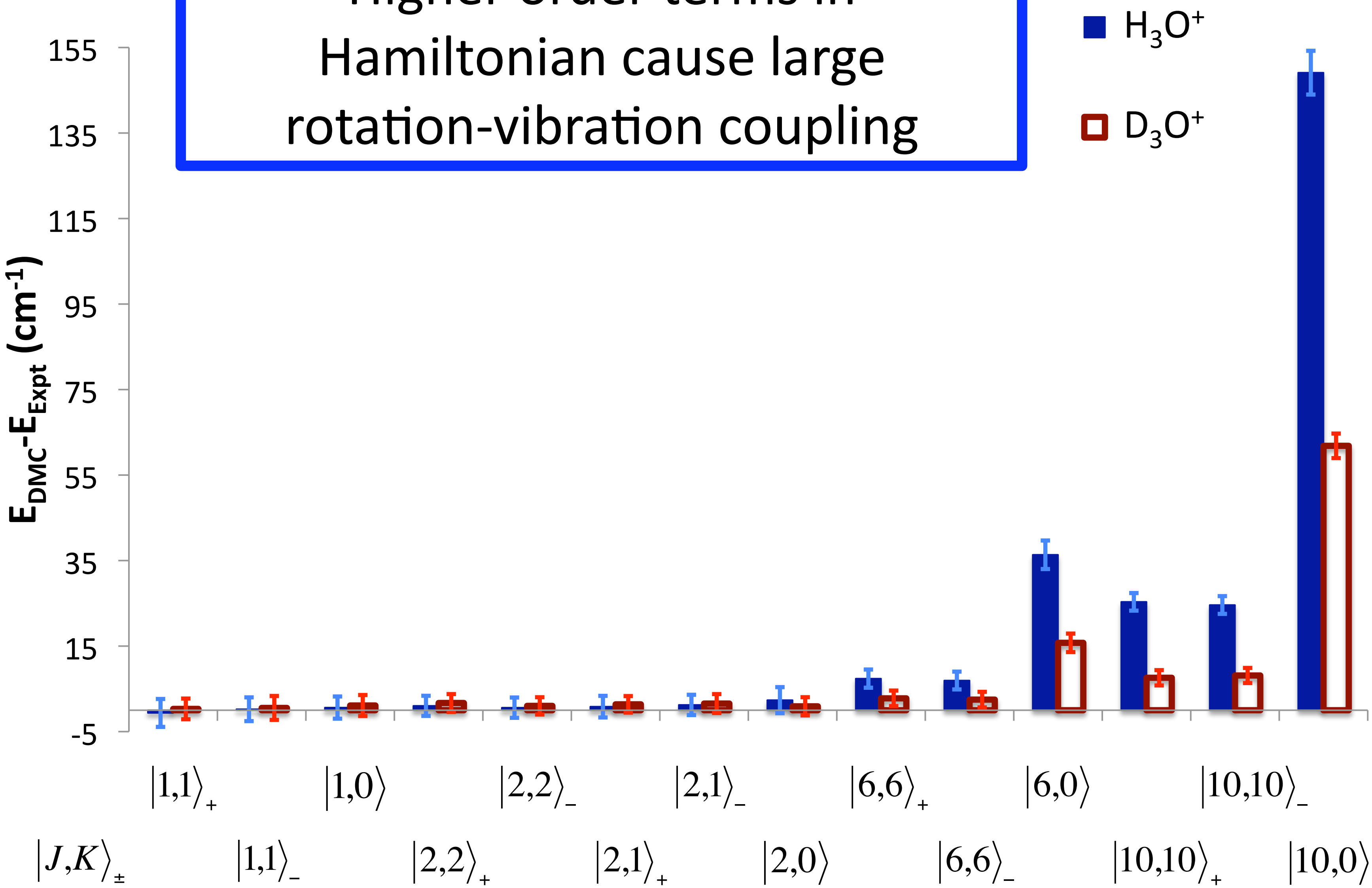
Higher order terms in Hamiltonian cause large rotation-vibration coupling



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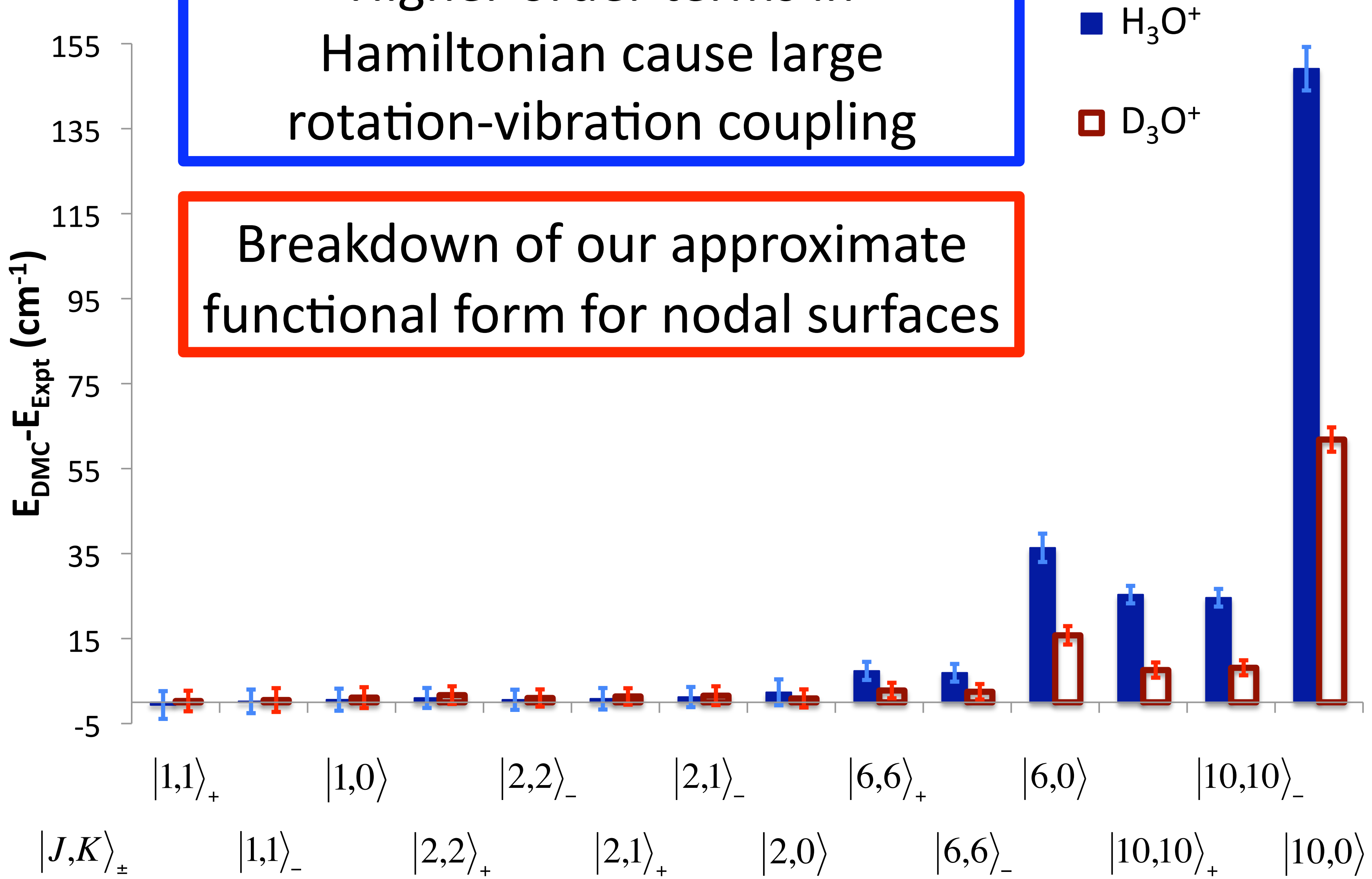

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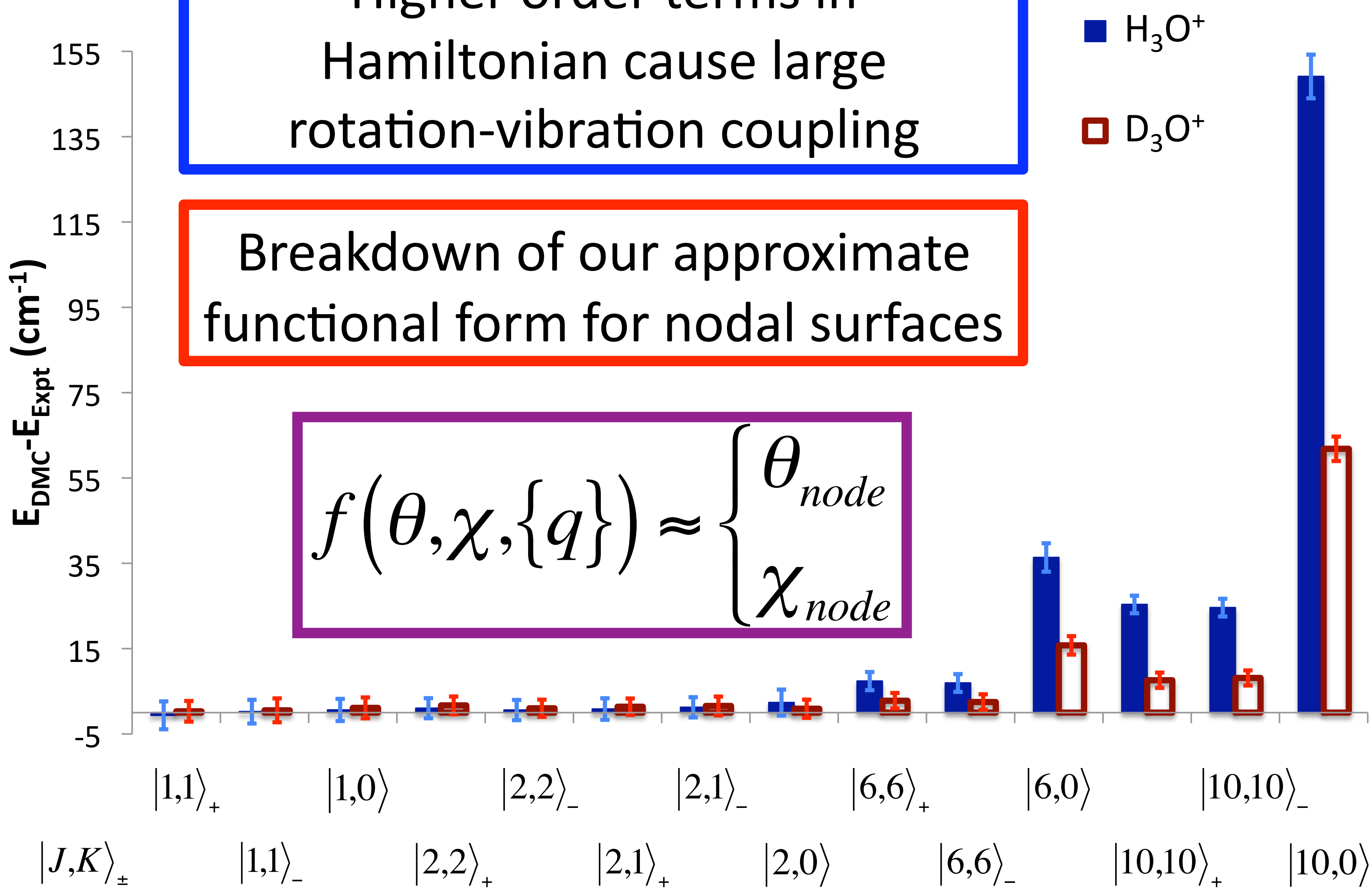

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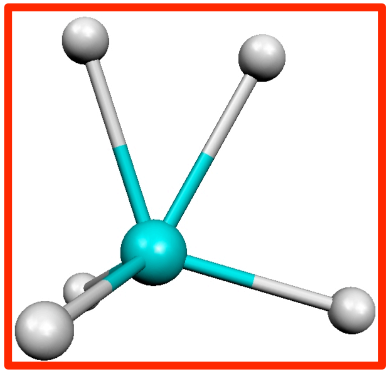

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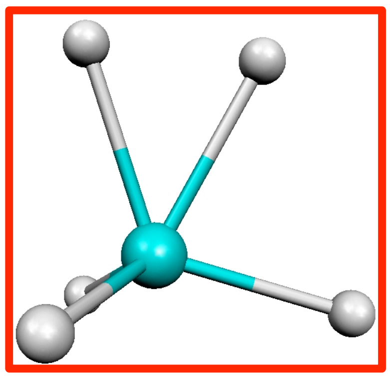
Study effects of rotational excitation on geometric structure

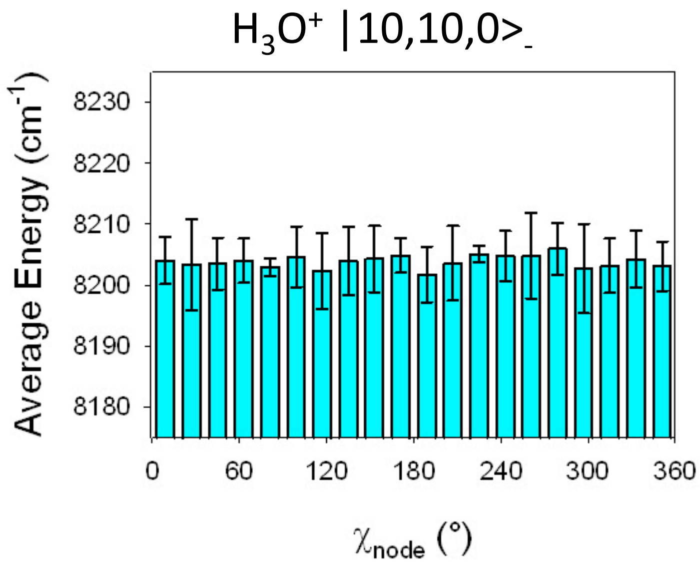
Some deviations at high J

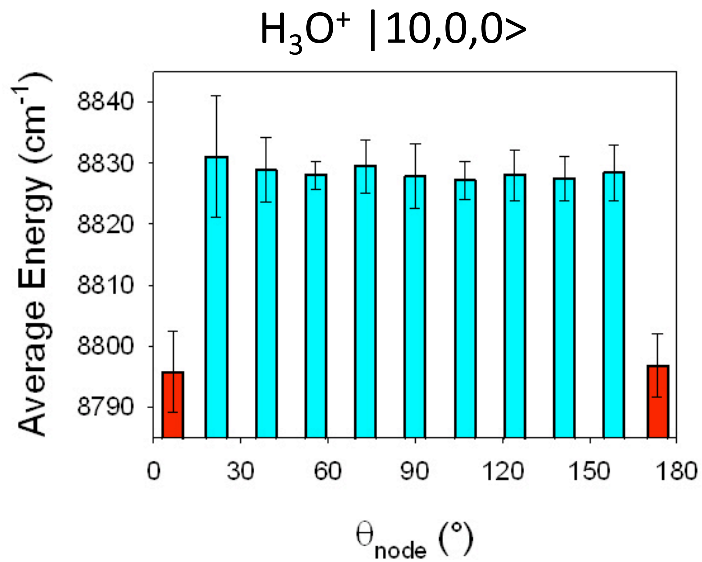


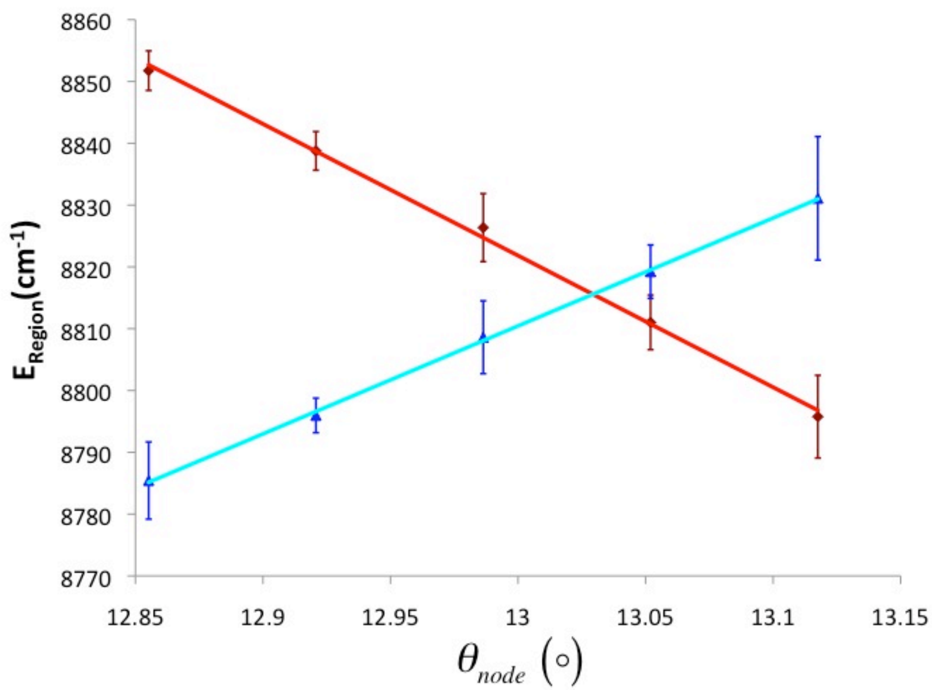
Generalization of approach to asymmetric tops

Acknowledgements

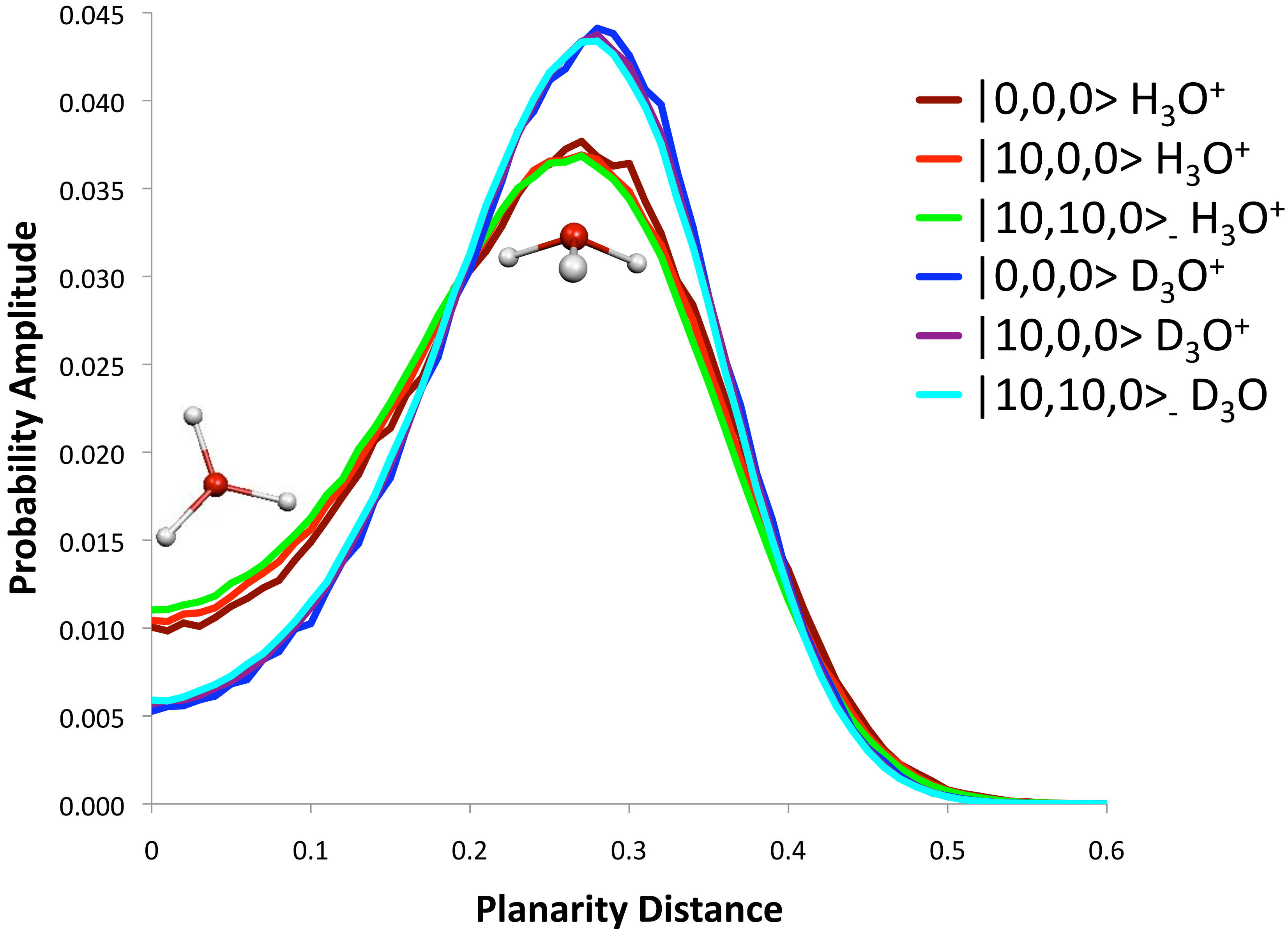
How Good Are Our Nodal Surfaces?



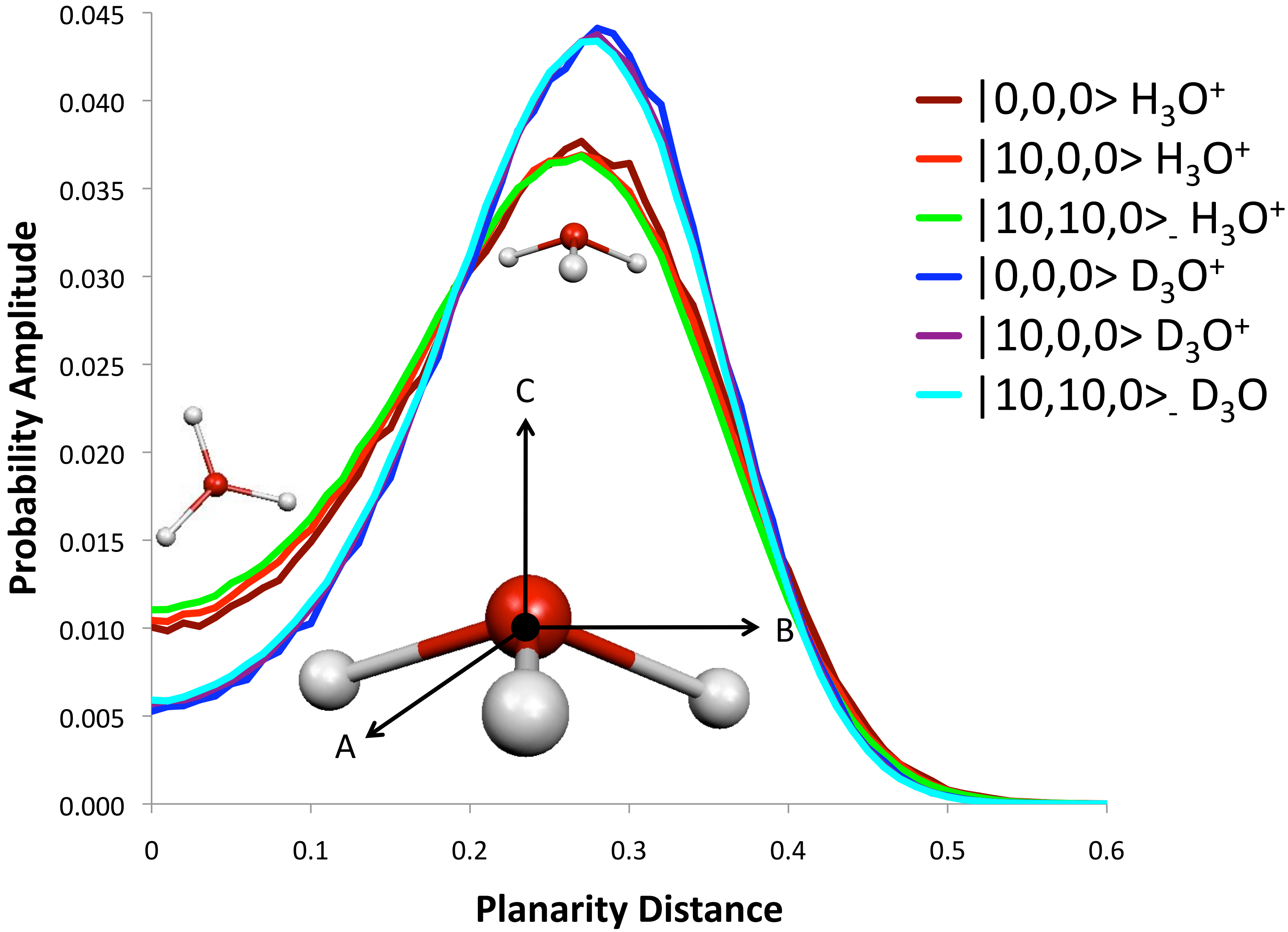




Probing Geometric Effects of Rotational Excitation with DMC



Probing Geometric Effects of Rotational Excitation with DMC

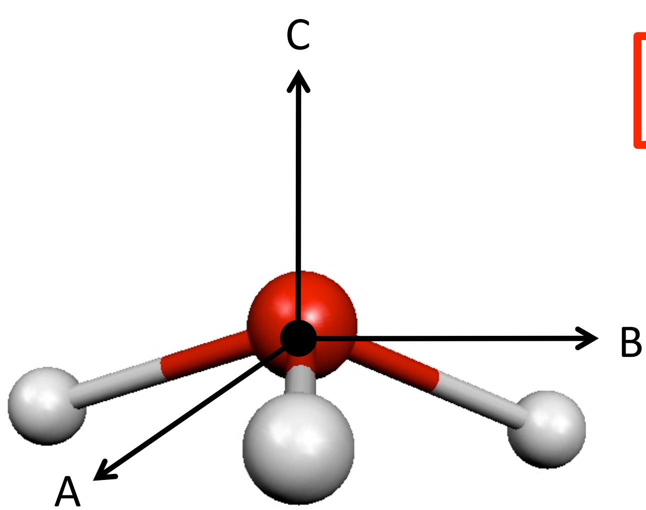


Probing Geometric Effects of Rotational Excitation with DMC

	H_3O^+		D_3O^+	
State	$\langle r_{OH} \rangle$(Å)	$\langle \theta_{HOH} \rangle$(°)	$\langle r_{OD} \rangle$(Å)	$\langle \theta_{DOD} \rangle$(°)
$\|0,0,0\rangle_+$	0.99564 ± 0.00026	113.062 ± 0.041	$0.99070 \pm .00020$	112.584 ± 0.031
$\|10,10,0\rangle_+$	0.00107 ± 0.00027	0.334 ± 0.043	0.00053 ± 0.00021	0.166 ± 0.032
$\|10,10,0\rangle_-$	0.00103 ± 0.00027	0.334 ± 0.043	0.00057 ± 0.00021	0.173 ± 0.032
$\|10,0,0\rangle$	$.00236 \pm 0.00029$	0.218 ± 0.045	0.00126 ± 0.00022	0.155 ± 0.034

Rotation about C axis:

Primarily affects molecular shape



Rotation about A OR B axes:

Larger impact on size

A Simple Game of Chance

$$\left|\Psi(\tau+\delta\tau)\right\rangle \cong e^{-(\hat{V}-\boxed{E_{ref}})\delta\tau} e^{-\hat{T}\delta\tau}\left|\Psi(\tau)\right\rangle$$

E_0 not known *a priori*

$$E_{ref}(\tau) = \boxed{\langle V(\tau)\rangle} - \alpha\left(\frac{\boxed{N(\tau)} - N(0)}{N(0)}\right)$$

Average potential energy of walkers

Instantaneous population of walkers

A Simple Game of Chance

$$e^{-\hat{T}\delta\tau}\delta^{3N}(\vec{x}-\vec{x}_i) \propto e^{-\frac{m_i(\vec{x}-\vec{x}_i)^2}{2\delta\tau}}$$

Diffusion of Walkers

Random Displacements in *ith*
Coordinate Taken from Gaussian of Width

$$\sigma_i = \sqrt{\frac{\delta\tau}{m_i}}$$

A Simple Game of Chance

$$e^{-\hat{T}\delta\tau}\delta^{3N}(\vec{x}-\vec{x}_i) = Ke^{-\frac{m_i(\vec{x}-\vec{x}_i)^2}{2\delta\tau}}$$

Diffusion of Walkers

Random Displacements in *ith* Coordinate Taken from Gaussian of Width

$$\sigma_i = \sqrt{\frac{\delta\tau}{m_i}}$$

A Simple Game of Chance

We Already Have the Wave Function

$$\Psi(\vec{x},\tau) \propto \sum_{i=1}^{N(\tau)} \delta^{3N}\left(\vec{x} - \vec{x}_i(\tau)\right)$$

GOAL:

$$\left|\Psi\left(\vec{x},\tau\right)\right|^2 \propto \sum_{i=1}^{N(\tau)} w_i(\tau)\delta^{3N}\left(\vec{x} - \vec{x}_i(\tau)\right)$$

A Simple Game of Chance

IF

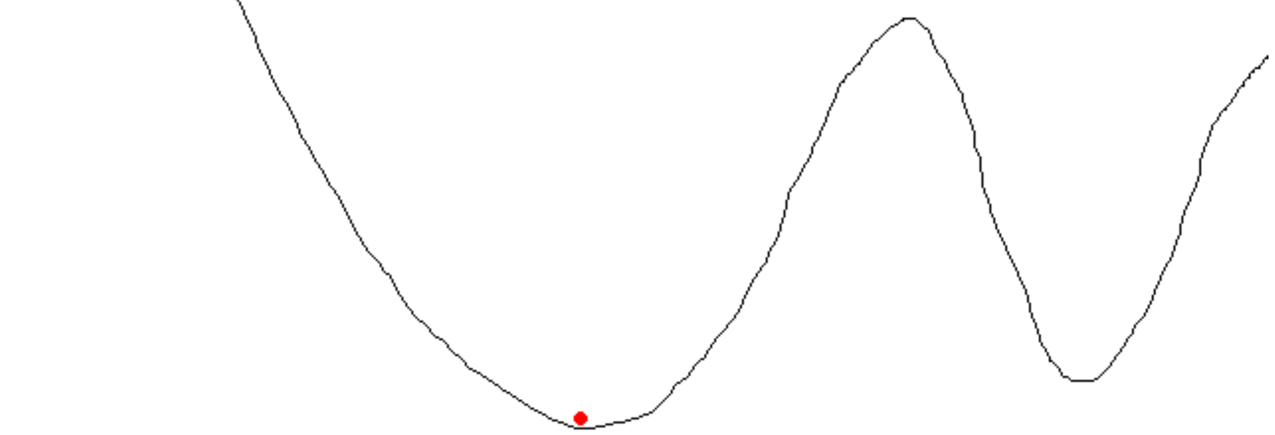
$$\left|\Psi\left(\vec{x},\tau\right)\right|^2 \propto \sum_{i=1}^{N(\tau)} w_i(\tau)\delta^{3N}\left(\vec{x}-\vec{x}_i(\tau)\right)$$

THEN

$$\left\langle A\right\rangle = \frac{\sum_{i=1}^{N(\tau)} w_i(\tau)A(\vec{x}_i)}{\sum_{i=1}^{N(\tau)} w_i(\tau)}$$

Descendent Weighting

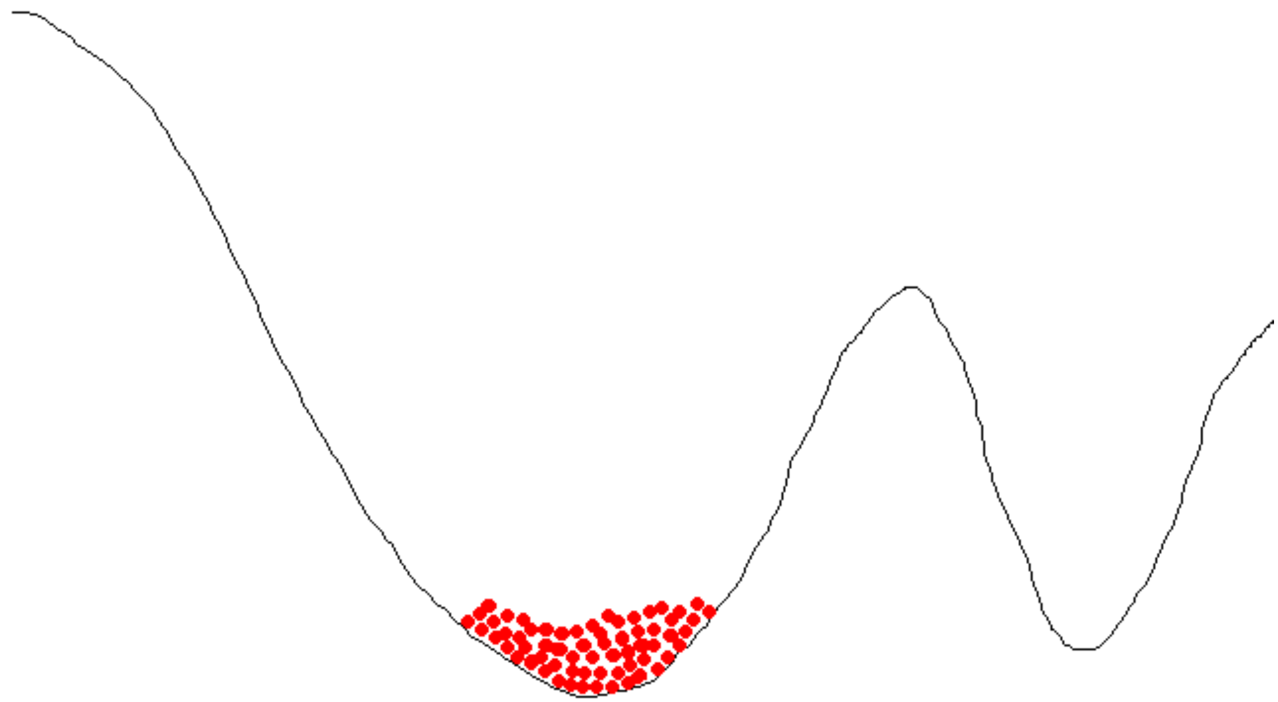
Imaginary Time:
$\boldsymbol{\tau}$



Descendent Weighting

Imaginary Time:

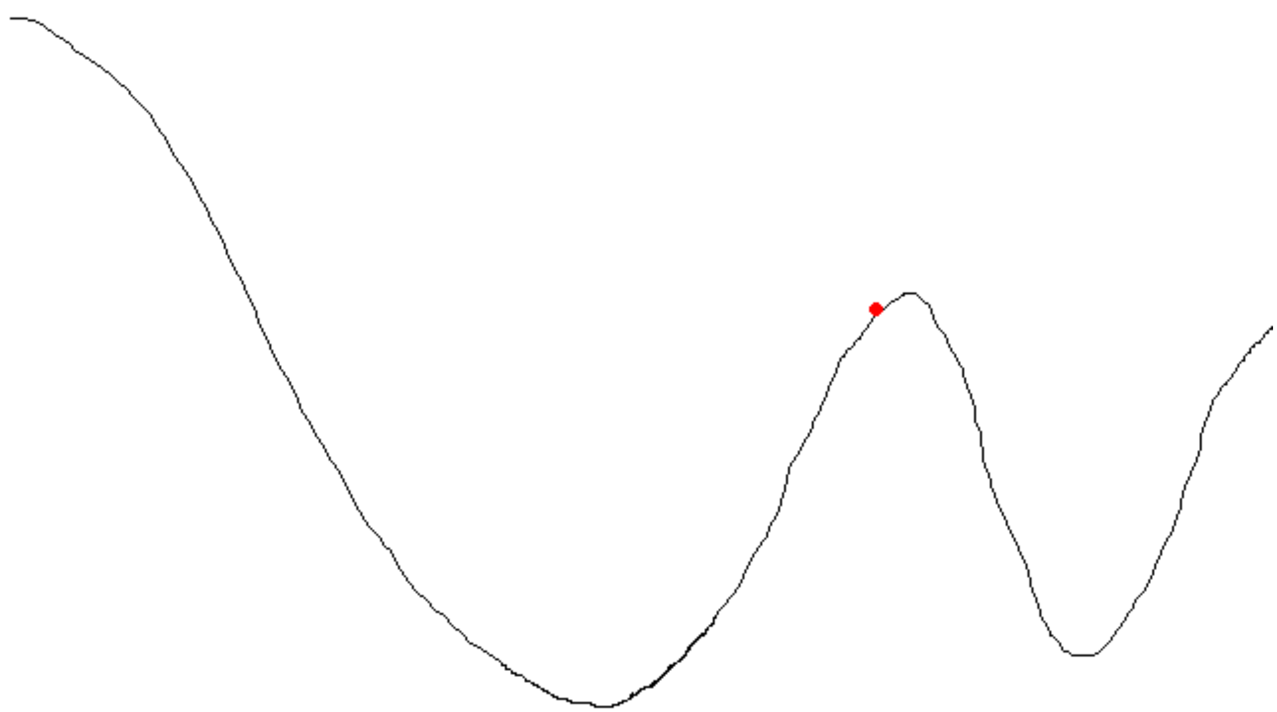
$$\tau + N_{step}$$



Descendent Weighting

Imaginary Time:

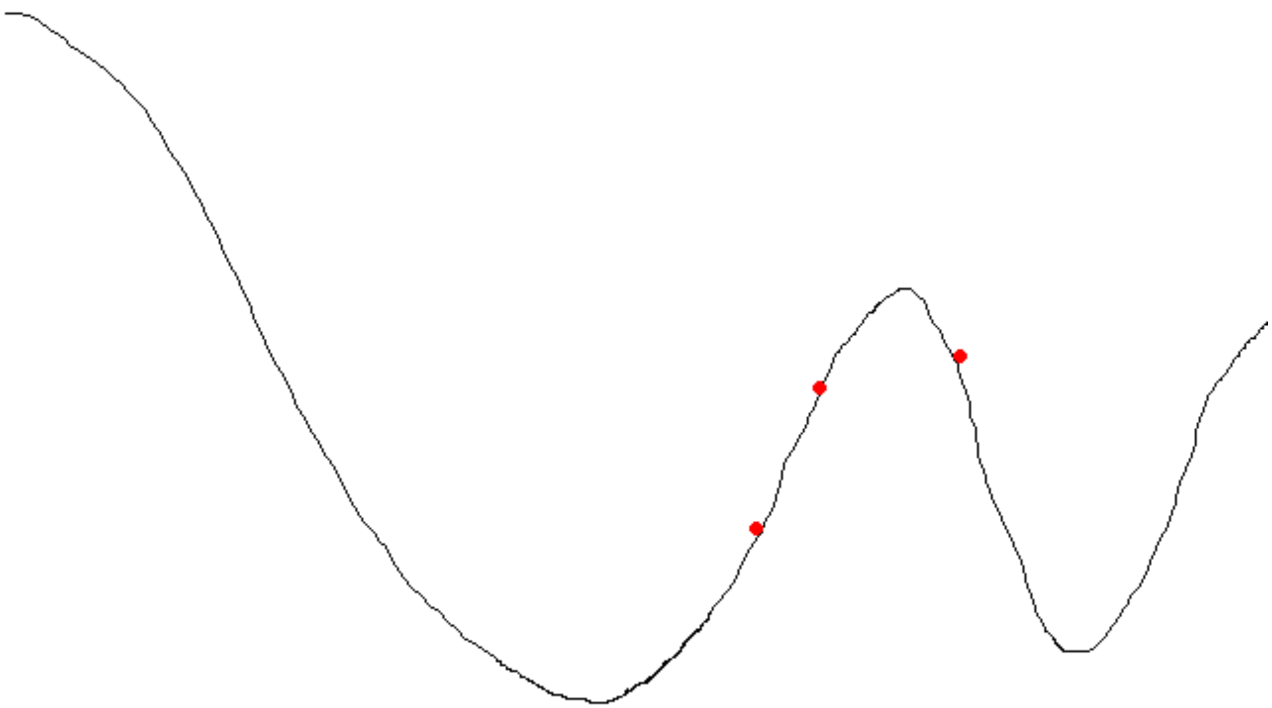
$\boldsymbol{\tau}$



Descendent Weighting

Imaginary Time:

$$\tau + N_{step}$$



Descendent Weighting

Imaginary Time:

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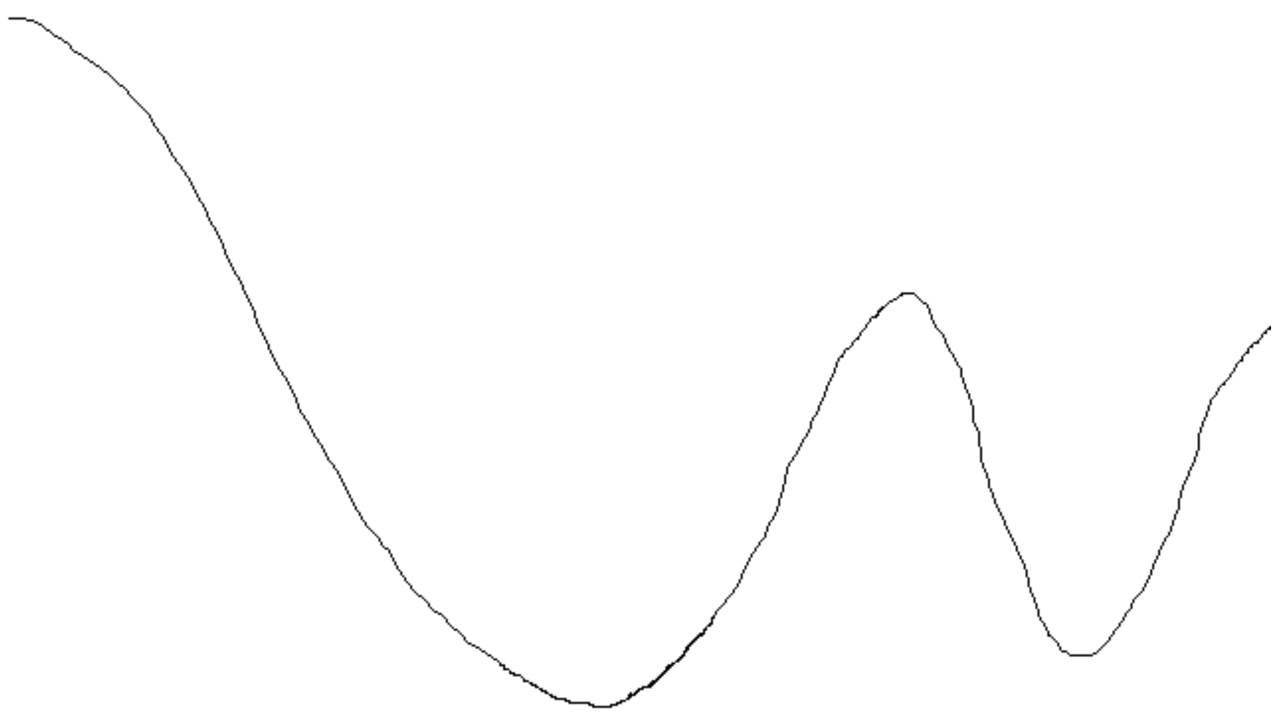
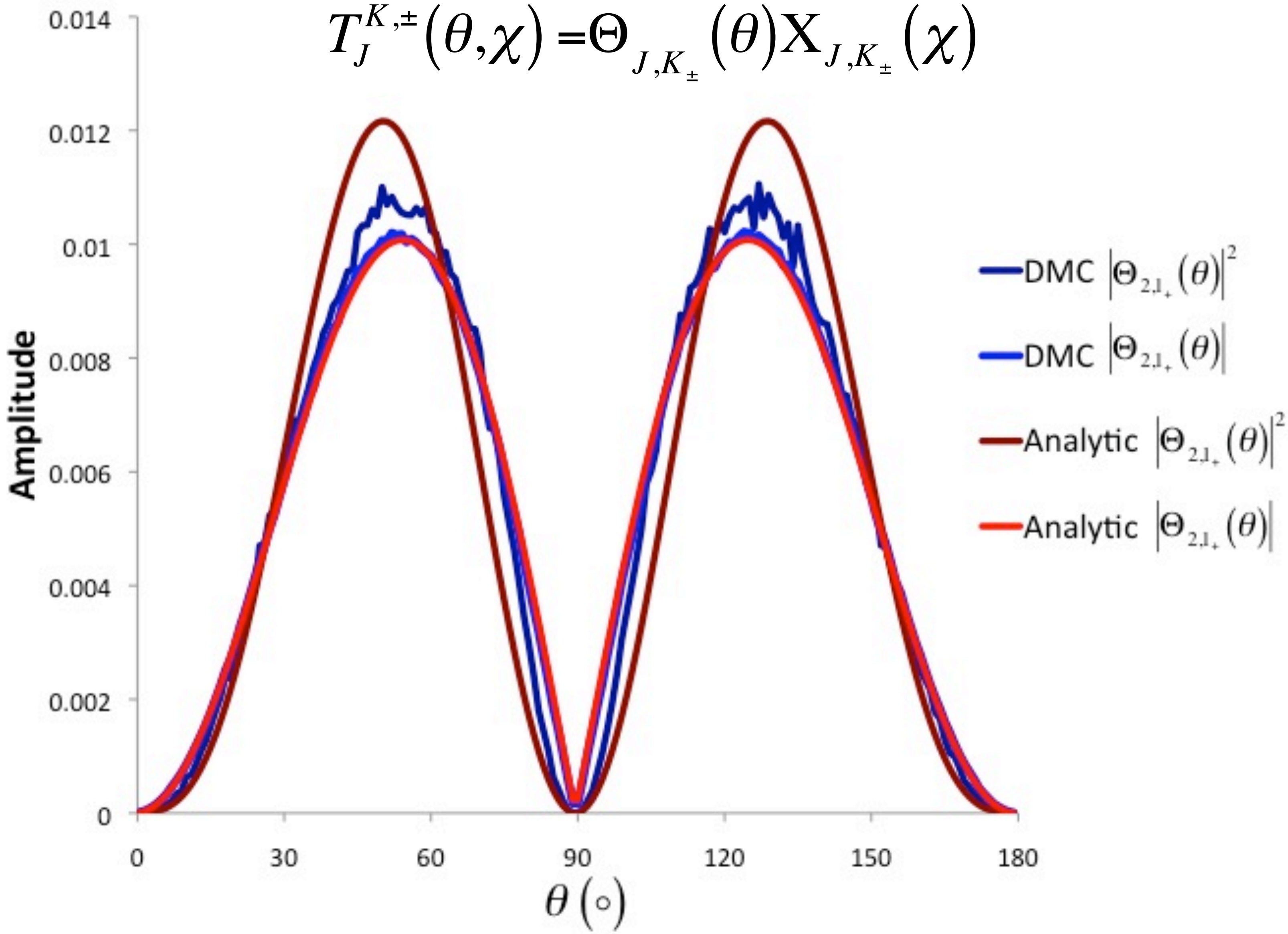
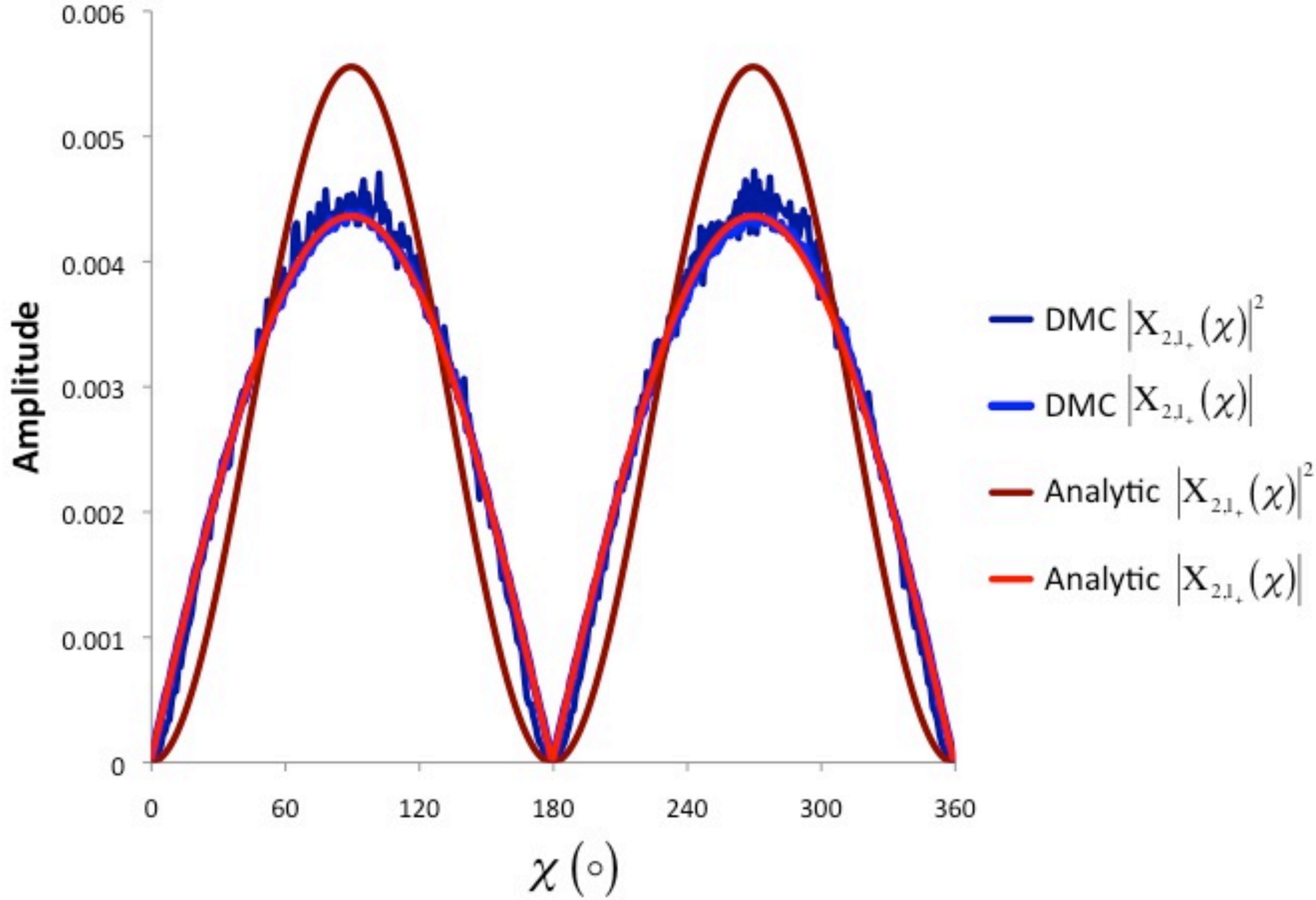


Projecting Wave Function onto Rotational Coordinates

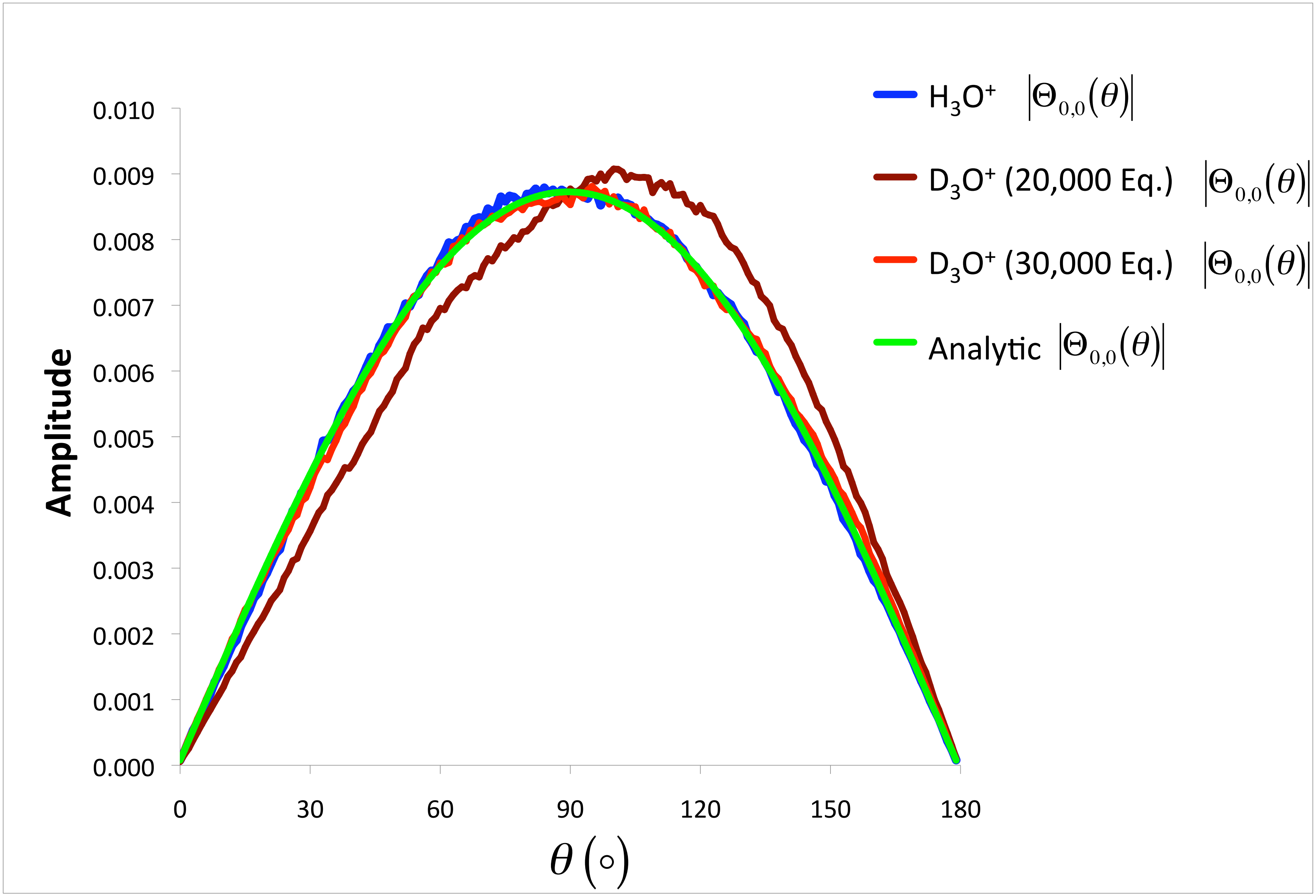
$$T_J^{K,\pm}(\theta,\chi) = \Theta_{J,K_\pm}(\theta)\mathrm{X}_{J,K_\pm}(\chi)$$



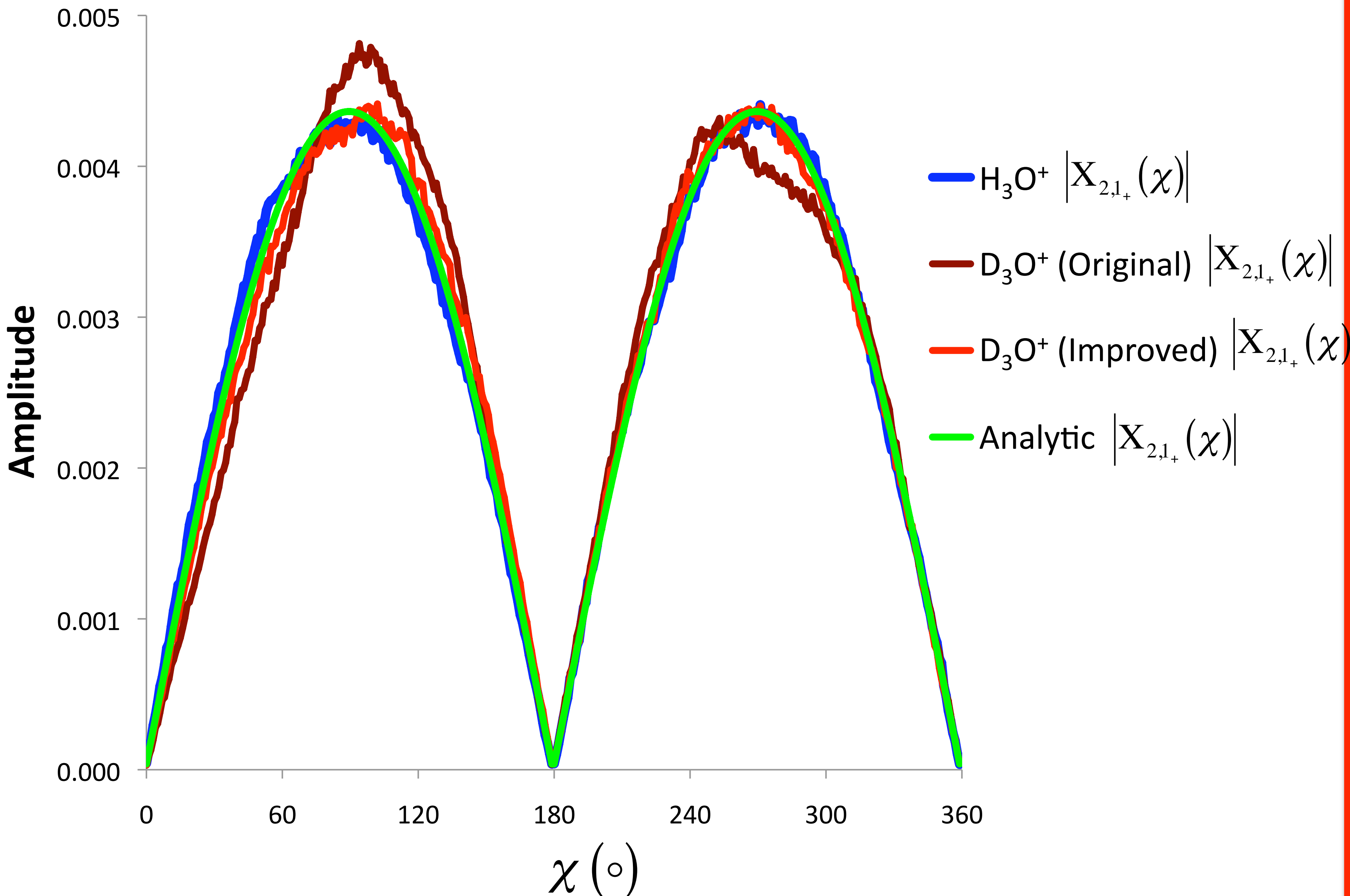
Projecting Wave Function onto Rotational Coordinates



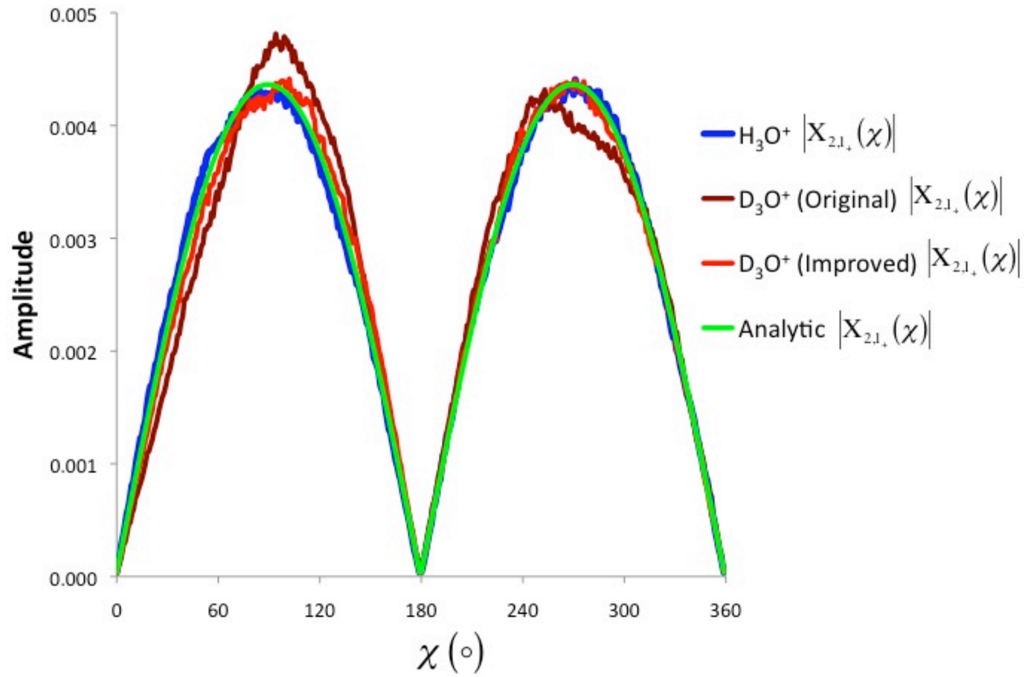
Monitoring Equilibration of Simulations



Monitoring Equilibration of Simulations



Monitoring Equilibration of Simulations



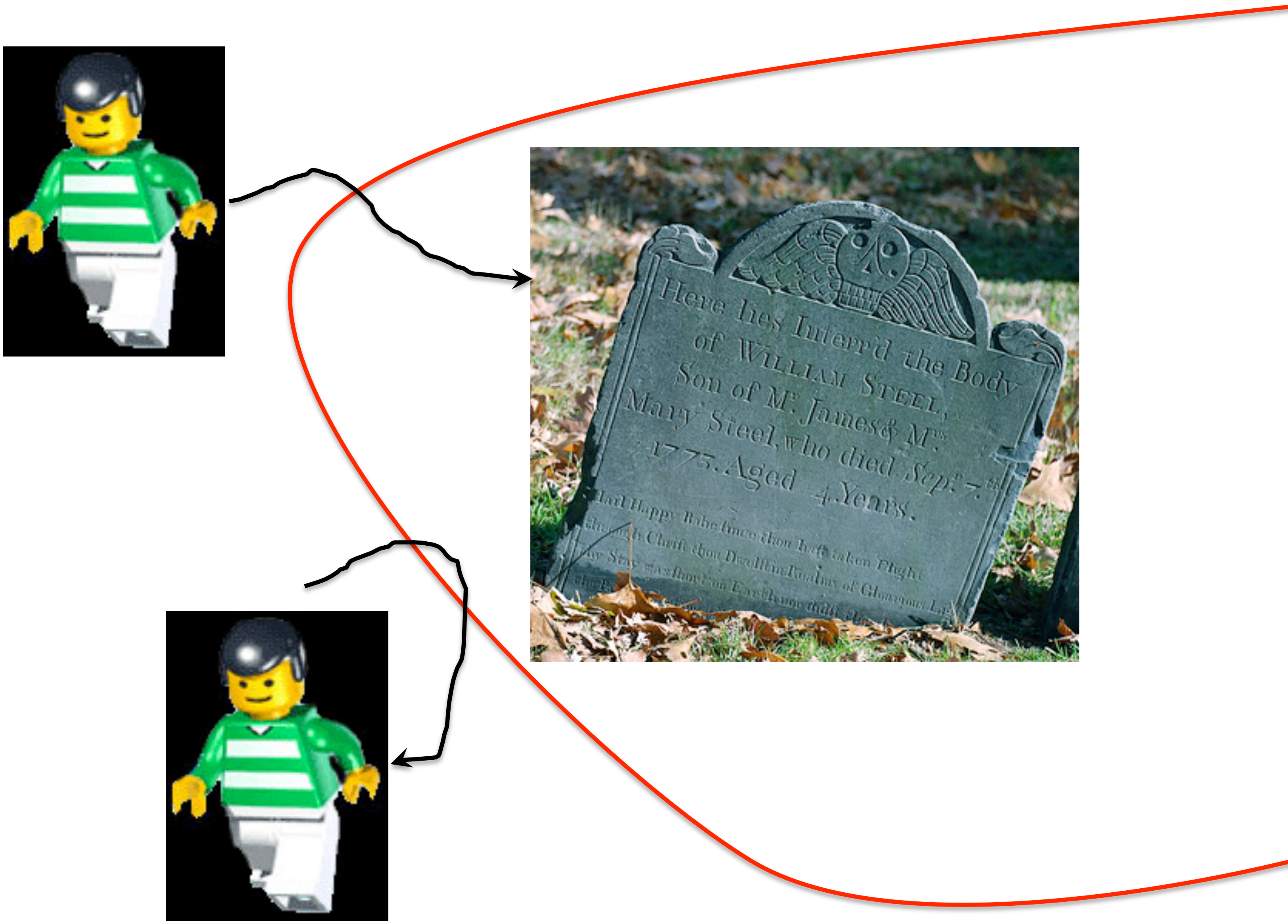
Only Observed for J≤1

Improvement to Projections Onto Rotational Coordinates Yielded Better Agreement With RVIB4 Energies

Better Indication of Equilibration Than Monitoring Energy

The Re-Crossing Correction

The Re-Crossing Correction



The Re-Crossing Correction

Probability of Walker Death Due to Node Re-Crossing:

$$P = Exp\left[\frac{-\boxed{d_i(\tau)}\,d_i(\tau+\delta\tau)\boxed{m_i}}{\delta\tau}\right]$$

Distance From *ith* Nodal Surface

Effective Mass Associated With *ith* Nodal Surface

$$d_i(\tau) = \theta(\tau) - \theta_{node}$$

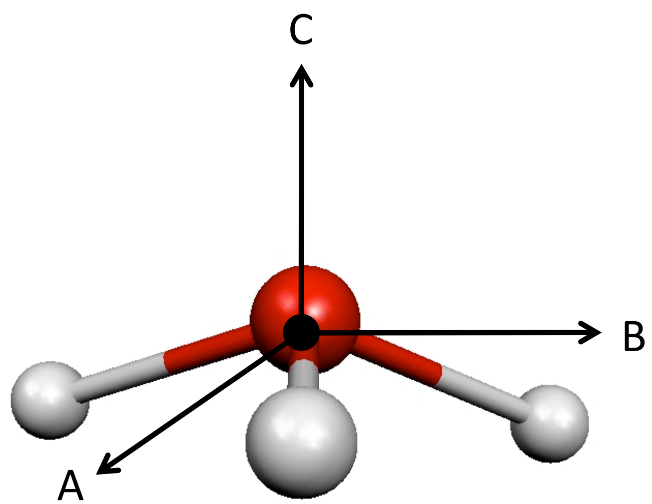
OR

$$d_i(\tau) = \chi(\tau) - \chi_{node}$$

Effective Masses for Symmetric Tops

$$\boxed{\theta = \theta_{node}}$$

$$\boxed{m_i = \sqrt{\left(\frac{I_A(\tau) + I_A(\tau + \delta\tau)}{2}\right)\left(\frac{I_B(\tau) + I_B(\tau + \delta\tau)}{2}\right)}}$$



$$\boxed{\chi = \chi_{node}}$$

$$\boxed{m_i = \frac{I_C(\tau) + I_C(\tau + \delta\tau)}{2}}$$